Quantum Mechanics I

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Contents

Part I

Mathematical and Physical Foundations

Chapter 1

Wave Functions, Vector Spaces, and Hilbert Space

1.1 The one-particle wave function

For a spinless nonrelativistic particle in three spatial dimensions, a state may be represented in the position basis by a complex wave function

$$\psi(\boldsymbol{r}, t) = \langle \boldsymbol{r} | \psi(t) \rangle \,. \tag{1.1}$$

The Born interpretation assigns the probability of finding the particle in a spatial region Ω at time t as

$$P(\Omega, t) = \int_{\Omega} |\psi(\boldsymbol{r}, t)|^2 \, \mathrm{d}^3 r. \tag{1.2}$$

For a normalizable state,

$$\int_{\mathbb{R}^3} |\psi(\boldsymbol{r}, t)|^2 \, \mathrm{d}^3 r = 1. \tag{1.3}$$

Thus ordinary wave functions belong to $L^2(\mathbb{R}^3)$, the space of square-integrable complex-valued functions. The statement $\psi : \mathbb{R}^3 \to \mathbb{C}$ is therefore only part of the story: physical states must satisfy the required regularity and normalizability conditions, and two state vectors differing only by an overall nonzero complex factor represent the same ray. Once a normalization convention is chosen, only an overall phase remains physically irrelevant.

Remark 1.1. Position and momentum eigenfunctions are not square-integrable. They are generalized vectors normalized with Dirac delta functions. A mathematically precise treatment uses a rigged Hilbert space; the standard Dirac formalism will be used here.

1.2 Complex vector spaces

A complex vector space V is a set equipped with vector addition and scalar multiplication by numbers in $\mathbb{C}$. If $|\psi\rangle, |\phi\rangle \in V$ and $a, b \in \mathbb{C}$, then

$$a |\psi\rangle + b |\phi\rangle \in V. \tag{1.4}$$

The usual vector-space axioms—associativity and commutativity of addition, existence of a zero vector and additive inverses, and distributive/associative rules for scalar multiplication—are assumed.

A set $\{|e_i\rangle\}$ is linearly independent if

$$\sum_i c_i \,|e_i\rangle = 0 \quad \implies \quad c_i = 0 \quad \text{for all } i. \tag{1.5}$$

It spans V if every vector in V can be expressed as a linear combination of its elements. A linearly independent spanning set is a basis.

1.3 Inner-product spaces

An inner product on a complex vector space is a map

$$V \times V \longrightarrow \mathbb{C}, \qquad (|\phi\rangle\,, |\psi\rangle) \mapsto \langle\phi|\psi\rangle\,, \tag{1.6}$$

with the following properties:

$$\langle\phi|a\psi + b\chi\rangle = a\,\langle\phi|\psi\rangle + b\,\langle\phi|\chi\rangle\,, \tag{1.7}$$

$$\langle a\phi + b\chi|\psi\rangle = a^*\,\langle\phi|\psi\rangle + b^*\,\langle\chi|\psi\rangle\,, \tag{1.8}$$

$$\langle\phi|\psi\rangle = \langle\psi|\phi\rangle^*\,, \tag{1.9}$$

$$\langle\psi|\psi\rangle \geq 0, \qquad \langle\psi|\psi\rangle = 0 \iff |\psi\rangle = 0. \tag{1.10}$$

The induced norm is

$$\|\psi\| = \sqrt{\langle\psi|\psi\rangle}. \tag{1.11}$$

For wave functions,

$$\langle\phi|\psi\rangle = \int \phi^*(\boldsymbol{r})\psi(\boldsymbol{r})\,\mathrm{d}^3r. \tag{1.12}$$

1.4 Cauchy–Schwarz and triangle inequalities

Theorem 1.1 (Cauchy–Schwarz)**.** *For any $|\phi\rangle\,, |\psi\rangle$ in an inner-product space,*

$$|\,\langle\phi|\psi\rangle\,|^2 \leq \langle\phi|\phi\rangle\,\langle\psi|\psi\rangle\,. \tag{1.13}$$

Equality holds iff the two vectors are linearly dependent.

Proof. For arbitrary $\lambda \in \mathbb{C}$,

$$0 \leq \|\psi - \lambda\phi\|^2. \tag{1.14}$$

If $\phi \neq 0$, choose

$$\lambda = \frac{\langle\phi|\psi\rangle}{\langle\phi|\phi\rangle}. \tag{1.15}$$

Substitution gives

$$0 \leq \langle\psi|\psi\rangle - \frac{|\,\langle\phi|\psi\rangle\,|^2}{\langle\phi|\phi\rangle}, \tag{1.16}$$

which is the result. □

Corollary 1.1 (Triangle inequality)**.**

$$\|\phi + \psi\| \leq \|\phi\| + \|\psi\|. \tag{1.17}$$

Proof. Using Cauchy–Schwarz,

$$\|\phi + \psi\|^2 = \|\phi\|^2 + \|\psi\|^2 + 2\,\mathrm{Re}\,\langle\phi|\psi\rangle \tag{1.18}$$

$$\leq \|\phi\|^2 + \|\psi\|^2 + 2\|\phi\|\|\psi\| \tag{1.19}$$

$$= (\|\phi\| + \|\psi\|)^2. \tag{1.20}$$

□

1.5 Hilbert space

Definition 1.1. A Hilbert space $\mathcal{H}$ is a complex inner-product space that is complete with respect to the norm induced by its inner product. Completeness means that every Cauchy sequence converges to an element of $\mathcal{H}$.

The completeness requirement is essential. A complex vector space with an inner product is not automatically a Hilbert space.

Quantum-mechanical state vectors live in a Hilbert space, with generalized eigenvectors such as $|x\rangle$ and $|p\rangle$ treated in the standard Dirac extension of that space.

1.6 Discrete orthonormal bases

Let $\{|u_n\rangle\}$ be a complete orthonormal basis:

$$\langle u_m|u_n\rangle = \delta_{mn}. \tag{1.21}$$

Completeness is expressed by the resolution of the identity,

$$\sum_n |u_n\rangle\langle u_n| = \mathbb{I}. \tag{1.22}$$

Any state can then be expanded as

$$|\psi\rangle = \sum_n c_n \, |u_n\rangle \,, \qquad c_n = \langle u_n|\psi\rangle \,. \tag{1.23}$$

If $|\psi\rangle$ is normalized,

$$1 = \langle\psi|\psi\rangle = \sum_n |c_n|^2, \tag{1.24}$$

which is Parseval's relation in this setting.

1.7 Continuous orthonormal bases and the Dirac delta

A continuum-labelled basis $\{|\alpha\rangle\}$ obeys

$$\langle\alpha|\alpha'\rangle = \delta(\alpha - \alpha') \tag{1.25}$$

and

$$\int \mathrm{d}\alpha \; |\alpha\rangle\langle\alpha| = \mathbb{I}. \tag{1.26}$$

Consequently,

$$|\psi\rangle = \int \mathrm{d}\alpha \; |\alpha\rangle \, \langle\alpha|\psi\rangle \,. \tag{1.27}$$

The Dirac delta is a distribution characterized by

$$\int_{-\infty}^{\infty} f(x)\delta(x-a)\,\mathrm{d}x = f(a), \tag{1.28}$$

with useful identities

$$\delta(x-a) = \delta(a-x), \tag{1.29}$$

$$\delta(cx) = \frac{1}{|c|}\delta(x), \tag{1.30}$$

$$\delta[f(x)] = \sum_i \frac{\delta(x - x_i)}{|f'(x_i)|}, \qquad f(x_i) = 0, \quad f'(x_i) \neq 0. \tag{1.31}$$

A Fourier representation is

$$\delta(x - x') = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}k(x-x')}\,\mathrm{d}k = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}p(x-x')/\hbar}\,\mathrm{d}p. \tag{1.32}$$

1.8 Plane waves and Fourier transforms

With the convention

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}}\,\mathrm{e}^{\mathrm{i}px/\hbar}, \tag{1.33}$$

we have

$$\langle p|p'\rangle = \delta(p - p'), \qquad \langle x|x'\rangle = \delta(x - x'). \tag{1.34}$$

The position- and momentum-space wave functions are related by

$$\psi(x) = \langle x|\psi\rangle = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} \phi(p)\mathrm{e}^{\mathrm{i}px/\hbar}\,\mathrm{d}p, \tag{1.35}$$

$$\phi(p) = \langle p|\psi\rangle = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} \psi(x)\mathrm{e}^{-\mathrm{i}px/\hbar}\,\mathrm{d}x. \tag{1.36}$$

Parseval's identity gives

$$\int |\psi(x)|^2\,\mathrm{d}x = \int |\phi(p)|^2\,\mathrm{d}p. \tag{1.37}$$

In three dimensions,

$$\langle \boldsymbol{r}|\boldsymbol{p}\rangle = \frac{1}{(2\pi\hbar)^{3/2}}\mathrm{e}^{\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{r}/\hbar}, \tag{1.38}$$

with

$$\int \mathrm{d}^3r\ |\boldsymbol{r}\rangle\langle\boldsymbol{r}| = \mathbb{I}, \qquad \int \mathrm{d}^3p\ |\boldsymbol{p}\rangle\langle\boldsymbol{p}| = \mathbb{I}. \tag{1.39}$$

1.9 Discrete and continuous labels together

A Hilbert space may contain both discrete and continuous labels. If $|n, \alpha\rangle$ denotes such a basis, then completeness takes the form

$$\sum_n \int \mathrm{d}\alpha\ |n, \alpha\rangle\langle n, \alpha| = \mathbb{I}, \tag{1.40}$$

with

$$\langle n, \alpha|m, \beta\rangle = \delta_{nm}\delta(\alpha - \beta). \tag{1.41}$$

This notation will reappear for angular momentum, spin, and scattering-type bases.

Chapter 2

Bras, Kets, Operators, and Representations

2.1 State space and dual space

A state vector is written as a ket $|\psi\rangle \in \mathcal{H}$. Its dual vector is a bra $\langle\psi| \in \mathcal{H}^*$, where $\mathcal{H}^*$ is the dual space of continuous linear functionals on $\mathcal{H}$. The map from kets to bras is antilinear:

$$a\,|\psi\rangle + b\,|\phi\rangle \quad \longmapsto \quad a^*\,\langle\psi| + b^*\,\langle\phi|\,. \tag{2.1}$$

Thus

$$(a\,|\psi\rangle + b\,|\phi\rangle)^\dagger = a^*\,\langle\psi| + b^*\,\langle\phi|\,. \tag{2.2}$$

The scalar product is the action of a bra on a ket:

$$\langle\phi|\,|\psi\rangle = \langle\phi|\psi\rangle\,. \tag{2.3}$$

2.2 Outer products

The outer product

$$|\psi\rangle\langle\phi| \tag{2.4}$$

is an operator. Acting on $|\chi\rangle$,

$$|\psi\rangle\langle\phi|\,|\chi\rangle = |\psi\rangle\,\langle\phi|\chi\rangle\,. \tag{2.5}$$

The adjoint is

$$(|\psi\rangle\langle\phi|)^\dagger = |\phi\rangle\langle\psi|\,. \tag{2.6}$$

If $|\psi\rangle$ is normalized, then

$$P_\psi = |\psi\rangle\langle\psi| \tag{2.7}$$

is an orthogonal projector:

$$P_\psi^2 = P_\psi, \qquad P_\psi^\dagger = P_\psi. \tag{2.8}$$

For a non-normalized vector,

$$|\psi\rangle\langle\psi| \tag{2.9}$$

is not idempotent unless $\langle\psi|\psi\rangle = 1$. The normalized rank-one projector is

$$P_\psi = \frac{|\psi\rangle\langle\psi|}{\langle\psi|\psi\rangle}. \tag{2.10}$$

2.3 Linear operators

A linear operator $\hat{A}$ satisfies

$$\hat{A}\left(a\left|\psi\right\rangle + b\left|\phi\right\rangle\right) = a\hat{A}\left|\psi\right\rangle + b\hat{A}\left|\phi\right\rangle. \tag{2.11}$$

Products of operators are generally noncommutative:

$$\hat{A}\hat{B} \neq \hat{B}\hat{A}. \tag{2.12}$$

The commutator and anticommutator are

$$\left[\hat{A},\hat{B}\right] = \hat{A}\hat{B} - \hat{B}\hat{A}, \qquad \left\{\hat{A},\hat{B}\right\} = \hat{A}\hat{B} + \hat{B}\hat{A}. \tag{2.13}$$

Useful identities include

$$[A, BC] = [A, B]\, C + B\, [A, C], \tag{2.14}$$

$$[AB, C] = A\, [B, C] + [A, C]\, B, \tag{2.15}$$

$$[A, [B, C]] + [B, [C, A]] + [C, [A, B]] = 0. \tag{2.16}$$

The last line is the Jacobi identity.

2.4 Adjoint and Hermitian conjugation

The adjoint $\hat{A}^\dagger$ is defined by

$$\left\langle\phi\middle|\hat{A}\middle|\psi\right\rangle = \left\langle\psi\middle|\hat{A}^\dagger\middle|\phi\right\rangle^* \tag{2.17}$$

for all suitable $\left|\phi\right\rangle, \left|\psi\right\rangle$. Equivalently,

$$\left\langle\phi\middle|\hat{A}\psi\right\rangle = \left\langle\hat{A}^\dagger\phi\middle|\psi\right\rangle. \tag{2.18}$$

Important rules are

$$(A + B)^\dagger = A^\dagger + B^\dagger, \tag{2.19}$$

$$(cA)^\dagger = c^* A^\dagger, \tag{2.20}$$

$$(AB)^\dagger = B^\dagger A^\dagger, \tag{2.21}$$

$$(A^{-1})^\dagger = (A^\dagger)^{-1}, \tag{2.22}$$

$$(A^\dagger)^\dagger = A. \tag{2.23}$$

Definition 2.1. An operator is Hermitian (self-adjoint in the finite-dimensional setting) if

$$A^\dagger = A. \tag{2.24}$$

It is anti-Hermitian if

$$A^\dagger = -A. \tag{2.25}$$

It is normal if

$$\left[A, A^\dagger\right] = 0. \tag{2.26}$$

If A is Hermitian, then $\langle\psi|A|\psi\rangle$ is real. If A is anti-Hermitian, its expectation value is purely imaginary.

A common construction is

$$A + A^\dagger \quad \text{(Hermitian)}, \qquad \mathrm{i}(A - A^\dagger) \quad \text{(Hermitian)}, \tag{2.27}$$

whereas $\mathrm{i}(A + A^\dagger)$ is anti-Hermitian.

2.5 Matrix representation

Choose an orthonormal basis $\{|u_i\rangle\}$. The matrix of A is

$$A_{ij} = \langle u_i|A|u_j\rangle\,. \tag{2.28}$$

If

$$|\psi\rangle = \sum_j c_j\,|u_j\rangle\,, \tag{2.29}$$

then

$$A\,|\psi\rangle = \sum_i \left(\sum_j A_{ij}c_j\right)|u_i\rangle\,. \tag{2.30}$$

Thus operator action becomes ordinary matrix multiplication in a chosen basis.

For a matrix,

$$A^\dagger = (A^*)^T. \tag{2.31}$$

A Hermitian matrix satisfies

$$A_{ij} = A^*_{ji}. \tag{2.32}$$

2.6 Change of basis

Let S be the unitary matrix relating two orthonormal bases. If state-coordinate columns transform as

$$\boldsymbol{c}' = S^\dagger\boldsymbol{c}, \tag{2.33}$$

then the operator matrix transforms as

$$A' = S^\dagger AS. \tag{2.34}$$

The exact placement of S and $S^\dagger$ depends on whether one views S as an active transformation of states or a passive change of coordinates; the invariant statement is that matrix elements must represent the same linear map in the new basis.

2.7 Eigenvalues and eigenvectors

An eigenvector of A satisfies

$$A\,|a\rangle = a\,|a\rangle\,. \tag{2.35}$$

The number a is an eigenvalue. In a finite-dimensional basis,

$$\det(A - aI) = 0 \tag{2.36}$$

is the characteristic equation.

Theorem 2.1 (Spectral theorem, finite-dimensional form)**.** *A Hermitian operator has real eigenvalues and an orthonormal basis of eigenvectors. More generally, every normal operator is unitarily diagonalizable.*

If

$$A\,|a,n\rangle = a\,|a,n\rangle\,, \tag{2.37}$$

where n labels degeneracy, the eigenspace projector is

$$P_a = \sum_n |a, n\rangle\langle a, n| \,. \tag{2.38}$$

Then

$$A = \sum_a a P_a \tag{2.39}$$

for a purely discrete spectrum, with sums replaced or supplemented by integrals for continuous spectra.

2.8 Orthogonality of eigenvectors of Hermitian operators

Suppose

$$A\,|a\rangle = a\,|a\rangle\,, \qquad A\,|b\rangle = b\,|b\rangle\,, \tag{2.40}$$

with $A = A^\dagger$. Then

$$\langle a|A|b\rangle = b\,\langle a|b\rangle\,, \tag{2.41}$$

$$\langle a|A|b\rangle = a\,\langle a|b\rangle\,. \tag{2.42}$$

Hence

$$(a - b)\,\langle a|b\rangle = 0. \tag{2.43}$$

Therefore distinct eigenvalues imply orthogonality. Within a degenerate eigenspace, one may choose an orthonormal basis by Gram–Schmidt orthogonalization.

2.9 Commuting observables and common eigenvectors

If A and B are Hermitian and

$$[A, B] = 0, \tag{2.44}$$

then there exists an orthonormal basis consisting of simultaneous eigenvectors of both operators. A useful proof is to observe that B preserves each eigenspace of A:

$$A(B\,|a\rangle) = B(A\,|a\rangle) = a(B\,|a\rangle). \tag{2.45}$$

One then diagonalizes B inside every degenerate eigenspace of A.

The converse statement must be phrased carefully: if two operators share a complete basis of simultaneous eigenvectors, then they commute. Sharing only one or a few common eigenvectors does not imply that their commutator vanishes as an operator.

2.10 Complete sets of commuting observables

A complete set of commuting observables (CSCO) is a set

$$\{A_1, A_2, \ldots, A_k\} \tag{2.46}$$

whose members mutually commute and whose simultaneous eigenvalues uniquely label the basis states, up to physically irrelevant phase choices. Symbolically,

$$A_i\,|a_1, a_2, \ldots\rangle = a_i\,|a_1, a_2, \ldots\rangle\,. \tag{2.47}$$

Angular momentum provides the canonical example: J^2 and J_z form a CSCO for a single irreducible angular-momentum multiplet.

2.11 Projectors and subspaces

An orthogonal projector P satisfies

$$P^2 = P, \qquad P^\dagger = P. \tag{2.48}$$

Its eigenvalues are 0 and 1. If $\mathcal{S} \subset \mathcal{H}$ is spanned by orthonormal vectors $|s_i\rangle$, then

$$P_{\mathcal{S}} = \sum_i |s_i\rangle\langle s_i| \,. \tag{2.49}$$

The complementary projector is

$$Q = I - P, \qquad Q^2 = Q, \qquad PQ = QP = 0. \tag{2.50}$$

2.12 Trace

For a trace-class operator A,

$$\operatorname{Tr} A = \sum_n \langle u_n|A|u_n\rangle \,, \tag{2.51}$$

where $\{|u_n\rangle\}$ is any orthonormal basis. The trace is basis-independent and obeys

$$\operatorname{Tr}(A + B) = \operatorname{Tr} A + \operatorname{Tr} B, \tag{2.52}$$

$$\operatorname{Tr}(cA) = c \operatorname{Tr} A, \tag{2.53}$$

$$\operatorname{Tr}(AB) = \operatorname{Tr}(BA), \tag{2.54}$$

$$\operatorname{Tr}(U^\dagger AU) = \operatorname{Tr} A \tag{2.55}$$

for products for which the traces exist. More generally,

$$\operatorname{Tr}(A_1 A_2 \cdots A_n) \tag{2.56}$$

is invariant under cyclic permutations, not under arbitrary permutations.

For a rank-one operator,

$$\operatorname{Tr}\left(|\psi\rangle\langle\phi|\right) = \langle\phi|\psi\rangle \,. \tag{2.57}$$

2.13 Functions of operators

If A has spectral decomposition

$$A = \sum_a a P_a, \tag{2.58}$$

then

$$f(A) = \sum_a f(a) P_a. \tag{2.59}$$

For analytic functions one may also use a power series,

$$f(A) = \sum_{n=0}^{\infty} c_n A^n. \tag{2.60}$$

If A and B commute, then

$$\mathrm{e}^{A+B} = \mathrm{e}^A \mathrm{e}^B = \mathrm{e}^B \mathrm{e}^A. \tag{2.61}$$

Without commutativity this factorization is generally false.

A very useful identity is the Hadamard lemma,

$$\mathrm{e}^{A}B\mathrm{e}^{-A} = B + [A, B] + \frac{1}{2!}\,[A, [A, B]] + \cdots . \tag{2.62}$$

The Baker–Campbell–Hausdorff formula begins as

$$\log(\mathrm{e}^{A}\mathrm{e}^{B}) = A + B + \frac{1}{2}\,[A, B] + \frac{1}{12}\,[A, [A, B]] + \frac{1}{12}\,[B, [B, A]] + \cdots . \tag{2.63}$$

2.14 Unitary operators and infinitesimal generators

A unitary operator U satisfies

$$U^{\dagger}U = UU^{\dagger} = I. \tag{2.64}$$

It preserves inner products and norms:

$$\langle U\phi|U\psi\rangle = \langle \phi|\psi\rangle . \tag{2.65}$$

Every unitary operator can be written locally as

$$U(\epsilon) = \exp\left(-\frac{\mathrm{i}\epsilon}{\hbar}G\right) \tag{2.66}$$

with a Hermitian generator G. Infinitesimally,

$$U(\epsilon) = I - \frac{\mathrm{i}\epsilon}{\hbar}G + O(\epsilon^{2}). \tag{2.67}$$

If instead one writes $U = \mathrm{e}^{\epsilon K}$ without extracting the factor of $-\mathrm{i}$, then the generator K is anti-Hermitian. These are equivalent conventions.

Under a simultaneous unitary change of representation,

$$|\psi\rangle \mapsto U\,|\psi\rangle , \qquad A \mapsto UAU^{\dagger}, \tag{2.68}$$

expectation values are unchanged. This should be distinguished from an *active physical rotation of the state* while the laboratory observable is held fixed. For rotations we will use the convention

$$U(R) = \exp\left(-\frac{\mathrm{i}}{\hbar}\boldsymbol{\theta}\cdot\boldsymbol{J}\right), \tag{2.69}$$

for which a vector operator satisfies $U^{\dagger}(R)\boldsymbol{V}U(R) = R\boldsymbol{V}$. A passive change of basis uses the corresponding inverse convention.

2.15 Tensor-product Hilbert spaces

For two systems with spaces $\mathcal{H}_1$ and $\mathcal{H}_2$, the composite space is

$$\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2. \tag{2.70}$$

Product basis states are

$$|i, j\rangle = |i\rangle \otimes |j\rangle , \tag{2.71}$$

with inner product

$$\langle i, j|k, \ell\rangle = \langle i|k\rangle \, \langle j|\ell\rangle . \tag{2.72}$$

If A acts only on subsystem 1 and B only on subsystem 2,

$$A \to A \otimes I, \qquad B \to I \otimes B, \tag{2.73}$$

and these operators commute:

$$[A \otimes I, I \otimes B] = 0. \tag{2.74}$$

Not every vector in $\mathcal{H}_1 \otimes \mathcal{H}_2$ factors into a product state; nonfactorizable states are entangled.

Chapter 3

Position, Momentum, and Wave Mechanics

3.1 Position operator

In one dimension, generalized position eigenkets satisfy

$$\hat{x}\,|x\rangle = x\,|x\rangle\,, \qquad \langle x|x'\rangle = \delta(x-x'), \qquad \int_{-\infty}^{\infty} \mathrm{d}x\ |x\rangle\langle x| = I. \tag{3.1}$$

For a state $|\psi\rangle$,

$$\psi(x) = \langle x|\psi\rangle\,. \tag{3.2}$$

Then

$$\langle x|\hat{x}\psi\rangle = x\psi(x), \tag{3.3}$$

so the position operator acts by multiplication in the position representation.

In three dimensions,

$$\hat{\boldsymbol{r}}\,|\boldsymbol{r}\rangle = \boldsymbol{r}\,|\boldsymbol{r}\rangle\,, \qquad \langle \boldsymbol{r}|\boldsymbol{r}'\rangle = \delta^{(3)}(\boldsymbol{r}-\boldsymbol{r}'). \tag{3.4}$$

3.2 Momentum operator and translations

The canonical commutator is

$$[\hat{x},\hat{p}] = \mathrm{i}\hbar. \tag{3.5}$$

A finite translation by a is generated by momentum:

$$T(a) = \exp\left(-\frac{\mathrm{i}a\hat{p}}{\hbar}\right). \tag{3.6}$$

With the active convention,

$$T(a)\,|x\rangle = |x+a\rangle\,. \tag{3.7}$$

Equivalently, the wave function of the translated state is

$$\psi_a(x) = \langle x|T(a)\psi\rangle = \psi(x-a). \tag{3.8}$$

For infinitesimal a,

$$\psi(x-a) = \psi(x) - a\frac{\mathrm{d}\psi}{\mathrm{d}x} + O(a^2), \tag{3.9}$$

while

$$T(a) = I - \frac{\mathrm{i}a\hat{p}}{\hbar} + O(a^2). \tag{3.10}$$

Comparing the two gives

$$\boxed{\hat{p} = -\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}x}} \tag{3.11}$$

in the position representation. In three dimensions,

$$\boxed{\hat{\boldsymbol{p}} = -\mathrm{i}\hbar\boldsymbol{\nabla}}. \tag{3.12}$$

The momentum eigenfunction is therefore

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}}\mathrm{e}^{\mathrm{i}px/\hbar}. \tag{3.13}$$

3.3 Canonical commutation relations

For Cartesian coordinates,

$$[x_i, x_j] = 0, \qquad [p_i, p_j] = 0, \qquad [x_i, p_j] = \mathrm{i}\hbar\delta_{ij}. \tag{3.14}$$

For a sufficiently regular function $F(\boldsymbol{x})$,

$$[p_i, F(\boldsymbol{x})] = -\mathrm{i}\hbar\frac{\partial F}{\partial x_i}. \tag{3.15}$$

Likewise, for a sufficiently regular function $G(\boldsymbol{p})$,

$$[x_i, G(\boldsymbol{p})] = \mathrm{i}\hbar\frac{\partial G}{\partial p_i}. \tag{3.16}$$

In particular,

$$[x, p^n] = \mathrm{i}\hbar n p^{n-1}, \qquad [x^n, p] = \mathrm{i}\hbar n x^{n-1}. \tag{3.17}$$

3.4 The Hamiltonian and the Schrödinger equation

For a nonrelativistic particle in a scalar potential $V(\boldsymbol{r}, t)$,

$$\hat{H} = \frac{\hat{\boldsymbol{p}}^2}{2m} + V(\hat{\boldsymbol{r}}, t). \tag{3.18}$$

The state obeys the time-dependent Schrödinger equation

$$\boxed{\mathrm{i}\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle}. \tag{3.19}$$

In the position representation,

$$\boxed{\mathrm{i}\hbar\frac{\partial\psi(\boldsymbol{r}, t)}{\partial t} = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{r}, t)\right]\psi(\boldsymbol{r}, t)}. \tag{3.20}$$

If the Hamiltonian is time-independent and

$$\hat{H}|E\rangle = E|E\rangle, \tag{3.21}$$

then stationary solutions have the form

$$|\psi_E(t)\rangle = \mathrm{e}^{-\mathrm{i}Et/\hbar}\,|E\rangle\,, \tag{3.22}$$

and the spatial wave function obeys

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{r})\right]\psi_E(\boldsymbol{r}) = E\psi_E(\boldsymbol{r}). \tag{3.23}$$

3.5 Expectation values in the position representation

For a normalized state,

$$\langle x\rangle = \int x|\psi(x)|^2\,\mathrm{d}x. \tag{3.24}$$

For momentum,

$$\langle p\rangle = \int \psi^*(x)\left(-\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}x}\right)\psi(x)\,\mathrm{d}x, \tag{3.25}$$

provided the boundary terms required for Hermiticity vanish. More generally,

$$\langle A\rangle = \langle\psi|A|\psi\rangle\,. \tag{3.26}$$

3.6 Hermiticity of differential operators

The formal differential expression $-\mathrm{i}\hbar\,\mathrm{d}/\,\mathrm{d}x$ becomes a self-adjoint momentum operator only after its domain and boundary conditions are specified appropriately. Integration by parts gives

$$\int_a^b \phi^*(-\mathrm{i}\hbar\psi')\,\mathrm{d}x = [-\mathrm{i}\hbar\phi^*\psi]_a^b + \int_a^b(-\mathrm{i}\hbar\phi')^*\psi\,\mathrm{d}x. \tag{3.27}$$

The boundary term must vanish for states in the operator domain. Similar domain issues occur for all unbounded observables.

3.7 Probability density and probability current

For

$$\rho(\boldsymbol{r},t) = |\psi(\boldsymbol{r},t)|^2, \tag{3.28}$$

the Schrödinger equation and its complex conjugate imply

$$\frac{\partial\rho}{\partial t} + \boldsymbol{\nabla}\cdot\boldsymbol{J} = 0, \tag{3.29}$$

where

$$\boxed{\boldsymbol{J} = \frac{\hbar}{2m\mathrm{i}}\left(\psi^*\boldsymbol{\nabla}\psi - \psi\boldsymbol{\nabla}\psi^*\right) = \frac{\hbar}{m}\,\mathrm{Im}(\psi^*\boldsymbol{\nabla}\psi)}. \tag{3.30}$$

This continuity equation expresses conservation of total probability when there is no probability flux through the boundary of the physical domain.

For a one-dimensional superposition of energy eigenstates,

$$\psi(x,t) = \sum_n c_n\phi_n(x)\mathrm{e}^{-\mathrm{i}E_nt/\hbar}, \tag{3.31}$$

interference terms in $|\psi|^2$ oscillate with Bohr frequencies

$$\omega_{nm} = \frac{E_n - E_m}{\hbar}. \tag{3.32}$$

3.8 Parity

The parity operator Π reverses spatial coordinates:

$$\Pi |\boldsymbol{r}\rangle = |-\boldsymbol{r}\rangle . \tag{3.33}$$

Hence

$$(\Pi\psi)(\boldsymbol{r}) = \psi(-\boldsymbol{r}). \tag{3.34}$$

Parity is both Hermitian and unitary:

$$\Pi^\dagger = \Pi, \qquad \Pi^2 = I. \tag{3.35}$$

Therefore its eigenvalues are ± 1. Even states satisfy

$$\Pi |\psi_+\rangle = + |\psi_+\rangle , \tag{3.36}$$

and odd states satisfy

$$\Pi |\psi_-\rangle = - |\psi_-\rangle . \tag{3.37}$$

Position and momentum are odd under parity:

$$\Pi\hat{\boldsymbol{r}}\Pi = -\hat{\boldsymbol{r}}, \qquad \Pi\hat{\boldsymbol{p}}\Pi = -\hat{\boldsymbol{p}}. \tag{3.38}$$

An operator A is parity-even if

$$\Pi A \Pi = A \tag{3.39}$$

and parity-odd if

$$\Pi A \Pi = -A. \tag{3.40}$$

3.9 Parity selection rules

Suppose $|i\rangle$ and $|f\rangle$ are parity eigenstates with parities $\pi_i, \pi_f = \pm 1$ and A has definite parity $\eta_A = \pm 1$:

$$\Pi A \Pi = \eta_A A. \tag{3.41}$$

Then

$$\langle f|A|i\rangle = \left\langle f \middle| \Pi^2 A \Pi^2 \middle| i \right\rangle \tag{3.42}$$

$$= \pi_f \pi_i \eta_A \langle f|A|i\rangle . \tag{3.43}$$

Hence a nonzero matrix element requires

$$\boxed{\pi_f \pi_i \eta_A = 1}. \tag{3.44}$$

Thus an even operator connects states of the same parity, whereas an odd operator connects states of opposite parity.

3.10 Parity-symmetric potentials

If

$$V(-x) = V(x), \tag{3.45}$$

then

$$[H, \Pi] = 0. \tag{3.46}$$

In one-dimensional bound-state problems, nondegenerate energy eigenstates may therefore be chosen with definite parity. For a symmetric infinite well centered at the origin, the eigenfunctions alternate between even and odd parity.

3.11 Separable Hamiltonians and product states

Consider a Hamiltonian

$$H = H_1 \otimes I + I \otimes H_2. \tag{3.47}$$

If

$$H_1 |n\rangle = E_n^{(1)} |n\rangle, \qquad H_2 |m\rangle = E_m^{(2)} |m\rangle, \tag{3.48}$$

then

$$|n, m\rangle = |n\rangle \otimes |m\rangle \tag{3.49}$$

is an eigenstate of H with

$$E_{nm} = E_n^{(1)} + E_m^{(2)}. \tag{3.50}$$

Degeneracy can occur when distinct pairs (n, m) yield the same total energy. Symmetry is often the structural reason behind systematic degeneracies, but accidental degeneracies may also occur.

3.12 Example: degeneracy in a two-dimensional box

For a rectangular infinite well with side lengths a and b,

$$E_{n_x n_y} = \frac{\pi^2 \hbar^2}{2m} \left(\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} \right), \qquad n_x, n_y = 1, 2, \ldots. \tag{3.51}$$

If $a = b$, interchange symmetry $x \leftrightarrow y$ implies

$$E_{n_x n_y} = E_{n_y n_x}, \tag{3.52}$$

so states with $n_x \neq n_y$ occur in symmetry-related degenerate pairs. For unequal sides this systematic degeneracy is generally lifted, although isolated accidental coincidences can still occur for special aspect ratios.

Chapter 4

Postulates, Measurements, and Uncertainty

4.1 From classical variables to quantum operators

Classical mechanics describes a system by canonical coordinates q_i, p_i and a Hamiltonian

$$H(q_i, p_i, t), \tag{4.1}$$

with Hamilton's equations

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \qquad \dot{p}_i = -\frac{\partial H}{\partial q_i}. \tag{4.2}$$

The Poisson bracket of two classical observables is

$$\{A, B\}_{\text{PB}} = \sum_i \left(\frac{\partial A}{\partial q_i}\frac{\partial B}{\partial p_i} - \frac{\partial A}{\partial p_i}\frac{\partial B}{\partial q_i} \right). \tag{4.3}$$

Canonical quantization heuristically promotes

$$q_i \to \hat{q}_i, \qquad p_i \to \hat{p}_i, \qquad \{A, B\}_{\text{PB}} \to \frac{1}{\mathrm{i}\hbar}\left[\hat{A}, \hat{B}\right]. \tag{4.4}$$

This correspondence is useful but should not be interpreted as a globally consistent rule for arbitrary classical functions: operator-ordering ambiguities and the Groenewold–van Hove obstruction prevent a universal exact map preserving all Poisson brackets.

4.2 The postulates of quantum mechanics

A compact formulation sufficient for the present course is as follows.

Postulate 4.1 (States)**.** At a fixed time, the physical state of a closed quantum system is represented by a ray in a complex Hilbert space $\mathcal{H}$. A normalized representative $|\psi\rangle$ satisfies

$$\langle\psi|\psi\rangle = 1. \tag{4.5}$$

Postulate 4.2 (Observables)**.** Every ideal observable A is represented by a self-adjoint operator $\hat{A}$ on $\mathcal{H}$.

Postulate 4.3 (Measurement probabilities)**.** Let the spectral decomposition of A be

$$A = \sum_a a P_a \tag{4.6}$$

for a discrete spectrum. If the system is in state $|\psi\rangle$, the probability of obtaining the value a is

$$\boxed{p(a) = \langle\psi|P_a|\psi\rangle}. \tag{4.7}$$

For a nondegenerate eigenvalue,

$$P_a = |a\rangle\langle a|\,, \qquad p(a) = |\,\langle a|\psi\rangle\,|^2. \tag{4.8}$$

For continuous spectra, probabilities are obtained from the spectral measure; for example, in the position basis,

$$P(x \in \Omega) = \int_\Omega |\psi(x)|^2 \, \mathrm{d}x. \tag{4.9}$$

Postulate 4.4 (State update for an ideal projective measurement)**.** If a measurement of A yields the result a, then immediately after an ideal projective measurement the state is

$$|\psi\rangle \longrightarrow \frac{P_a\,|\psi\rangle}{\sqrt{\langle\psi|P_a|\psi\rangle}}. \tag{4.10}$$

For a nondegenerate eigenvalue this reduces, up to a phase, to the eigenstate $|a\rangle$.

Postulate 4.5 (Time evolution)**.** For a closed system, time evolution is unitary and generated by the Hamiltonian:

$$\mathrm{i}\hbar \frac{\mathrm{d}}{\mathrm{d}t}\,|\psi(t)\rangle = H(t)\,|\psi(t)\rangle\,. \tag{4.11}$$

4.3 Expectation values and statistical moments

Repeated measurements of A on identically prepared systems produce a distribution of outcomes. The expectation value is

$$\boxed{\langle A\rangle = \langle\psi|A|\psi\rangle} \tag{4.12}$$

for a pure normalized state. If

$$A = \sum_a a P_a, \tag{4.13}$$

then

$$\langle A\rangle = \sum_a a\,p(a). \tag{4.14}$$

The variance is

$$(\Delta A)^2 = \left\langle (A - \langle A\rangle)^2 \right\rangle = \langle A^2\rangle - \langle A\rangle^2. \tag{4.15}$$

Hence

$$\Delta A = \sqrt{\langle A^2\rangle - \langle A\rangle^2}. \tag{4.16}$$

4.4 Discrete spectra and projectors

Suppose

$$|\psi\rangle = \sum_{a,r} c_{a,r} \, |a, r\rangle \, , \tag{4.17}$$

where r labels degeneracy. Then

$$p(a) = \sum_{r} |c_{a,r}|^2. \tag{4.18}$$

The post-measurement state conditioned on outcome a is

$$|\psi_a\rangle = \frac{\sum_r c_{a,r} \, |a, r\rangle}{\sqrt{\sum_r |c_{a,r}|^2}}. \tag{4.19}$$

Thus an ideal measurement of a degenerate eigenvalue projects into the full eigenspace, not necessarily onto one arbitrarily selected basis vector within that eigenspace.

4.5 Continuous measurements

If A has generalized eigenkets $|a\rangle$ with

$$\langle a|a'\rangle = \delta(a - a'), \tag{4.20}$$

then

$$\psi(a) = \langle a|\psi\rangle \tag{4.21}$$

is a probability amplitude and

$$p(a) = |\psi(a)|^2 \tag{4.22}$$

is a probability density. The probability in an interval is

$$P(a \in [a_1, a_2]) = \int_{a_1}^{a_2} |\psi(a)|^2 \, \mathrm{d}a. \tag{4.23}$$

One should distinguish a probability density from a probability itself.

4.6 Compatible observables and sequential measurements

Two observables are compatible when their spectral projectors commute; for ordinary finite-dimensional Hermitian operators this is equivalent to

$$[A, B] = 0. \tag{4.24}$$

They then possess a common orthonormal eigenbasis and can be assigned simultaneously sharp values in common eigenstates.

If A and B do not commute, the order of ideal projective measurements generally matters. If A is measured first with outcome a and then B with outcome b, the joint probability is

$$p(a \to b) = \langle \psi | P_a Q_b P_a | \psi \rangle \, , \tag{4.25}$$

where P_a and Q_b are the projectors associated with A and B. Reversing the order gives

$$p(b \to a) = \langle \psi | Q_b P_a Q_b | \psi \rangle \, , \tag{4.26}$$

which need not be equal.

4.7 Robertson uncertainty relation

Define centered operators

$$\widetilde{A} = A - \langle A \rangle, \qquad \widetilde{B} = B - \langle B \rangle. \tag{4.27}$$

Cauchy–Schwarz applied to

$$|\alpha\rangle = \widetilde{A}\,|\psi\rangle\,, \qquad |\beta\rangle = \widetilde{B}\,|\psi\rangle \tag{4.28}$$

gives

$$(\Delta A)^2(\Delta B)^2 \geq |\left\langle \psi \middle| \widetilde{A}\widetilde{B} \middle| \psi \right\rangle|^2. \tag{4.29}$$

Taking the imaginary part yields the Robertson bound

$$\boxed{\Delta A\,\Delta B \geq \frac{1}{2}\,|\langle [A,B] \rangle|}. \tag{4.30}$$

For position and momentum,

$$\boxed{\Delta x\,\Delta p \geq \frac{\hbar}{2}}. \tag{4.31}$$

4.8 Schrödinger uncertainty relation

Retaining both real and imaginary parts yields the stronger relation

$$(\Delta A)^2(\Delta B)^2 \geq \frac{1}{4}|\langle [A,B] \rangle|^2 + \frac{1}{4}\left|\left\langle \left\{ \widetilde{A}, \widetilde{B} \right\} \right\rangle\right|^2. \tag{4.32}$$

The anticommutator term is a covariance contribution. The Robertson relation follows immediately by discarding this nonnegative term.

4.9 When is the uncertainty zero?

For a normalized state,

$$\Delta A = 0 \tag{4.33}$$

if and only if $|\psi\rangle$ is an eigenstate of A. Indeed,

$$(\Delta A)^2 = \|\,(A - \langle A \rangle)\,|\psi\rangle\,\|^2, \tag{4.34}$$

which vanishes precisely when

$$A\,|\psi\rangle = \langle A \rangle\,|\psi\rangle\,. \tag{4.35}$$

4.10 Selection rules from symmetry

If G is a symmetry generator satisfying

$$[H, G] = 0, \tag{4.36}$$

then G is conserved under time evolution if it has no explicit time dependence. Matrix-element selection rules often follow from transformation properties of perturbing operators under the relevant symmetry. Parity selection rules were derived in the previous chapter; angular-momentum selection rules will be developed later using tensor operators and the Wigner–Eckart theorem.

Chapter 5

Time Evolution, Ehrenfest's Theorem, and Pictures of Motion

5.1 Unitary time evolution

The time-evolution operator is defined by

$$|\psi(t)\rangle = U(t,t_0)\,|\psi(t_0)\rangle\,. \tag{5.1}$$

It obeys

$$\mathrm{i}\hbar\frac{\partial U(t,t_0)}{\partial t} = H(t)U(t,t_0), \qquad U(t_0,t_0) = I. \tag{5.2}$$

Hermiticity of H implies unitarity of U:

$$U^\dagger(t,t_0)U(t,t_0) = I. \tag{5.3}$$

The composition law is

$$U(t_2,t_0) = U(t_2,t_1)U(t_1,t_0), \tag{5.4}$$

and

$$U(t_0,t) = U^{-1}(t,t_0) = U^\dagger(t,t_0). \tag{5.5}$$

If H is time-independent,

$$\boxed{U(t,t_0) = \exp\left[-\frac{\mathrm{i}H(t-t_0)}{\hbar}\right]}. \tag{5.6}$$

If $H(t)$ at different times does not commute with itself,

$$[H(t),H(t')] \neq 0, \tag{5.7}$$

one must use a time-ordered exponential,

$$U(t,t_0) = \mathcal{T}\exp\left[-\frac{\mathrm{i}}{\hbar}\int_{t_0}^{t} H(t')\,\mathrm{d}t'\right]. \tag{5.8}$$

5.2 Expansion in energy eigenstates

For a time-independent Hamiltonian with

$$H\,|n\rangle = E_n\,|n\rangle\,, \tag{5.9}$$

a general initial state

$$|\psi(0)\rangle = \sum_n c_n |n\rangle \tag{5.10}$$

evolves as

$$\boxed{|\psi(t)\rangle = \sum_n c_n \mathrm{e}^{-\mathrm{i}E_n t/\hbar} |n\rangle}. \tag{5.11}$$

The probabilities of measuring energy eigenvalues do not change:

$$|c_n(t)|^2 = |c_n(0)|^2. \tag{5.12}$$

Relative phases, however, evolve and can alter probabilities for other observables.

5.3 Global versus relative phase

Multiplication by a global phase,

$$|\psi\rangle \to \mathrm{e}^{\mathrm{i}\alpha} |\psi\rangle, \tag{5.13}$$

does not change any expectation value or measurement probability. By contrast, in a superposition

$$c_1 |1\rangle + c_2 \mathrm{e}^{\mathrm{i}\varphi} |2\rangle, \tag{5.14}$$

the relative phase φ is physically observable through interference with observables that connect the two components.

5.4 Ehrenfest theorem

For a possibly explicitly time-dependent operator $A(t)$,

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle A\rangle = \frac{\mathrm{d}}{\mathrm{d}t}\langle\psi(t)|A(t)|\psi(t)\rangle \tag{5.15}$$

$$= \left\langle \frac{\partial A}{\partial t} \right\rangle + \frac{\mathrm{i}}{\hbar}\langle [H, A]\rangle. \tag{5.16}$$

Equivalently,

$$\boxed{\frac{\mathrm{d}}{\mathrm{d}t}\langle A\rangle = \left\langle \frac{\partial A}{\partial t} \right\rangle + \frac{1}{\mathrm{i}\hbar}\langle [A, H]\rangle}. \tag{5.17}$$

These two forms are identical because $[H, A] = -[A, H]$.

For

$$H = \frac{p^2}{2m} + V(x), \tag{5.18}$$

we obtain

$$\frac{\mathrm{d}\langle x\rangle}{\mathrm{d}t} = \frac{\langle p\rangle}{m}, \tag{5.19}$$

$$\frac{\mathrm{d}\langle p\rangle}{\mathrm{d}t} = -\left\langle \frac{\mathrm{d}V}{\mathrm{d}x} \right\rangle. \tag{5.20}$$

Thus

$$m\frac{\mathrm{d}^2\langle x\rangle}{\mathrm{d}t^2} = -\langle V'(x)\rangle. \tag{5.21}$$

Only when $V'(x)$ is linear in x (or when fluctuations are negligible) does this reduce exactly to the classical equation evaluated at $\langle x\rangle$.

5.5 Driven harmonic oscillator at the level of expectation values

For

$$H = \frac{p^2}{2m} + \frac{1}{2}kx^2 + qE_0 x\cos\omega t, \tag{5.22}$$

Ehrenfest's theorem gives

$$\frac{\mathrm{d}\langle x\rangle}{\mathrm{d}t} = \frac{\langle p\rangle}{m}, \tag{5.23}$$

$$\frac{\mathrm{d}\langle p\rangle}{\mathrm{d}t} = -k\langle x\rangle - qE_0\cos\omega t. \tag{5.24}$$

Therefore

$$\boxed{\frac{\mathrm{d}^2\langle x\rangle}{\mathrm{d}t^2} + \omega_0^2\langle x\rangle = -\frac{qE_0}{m}\cos\omega t}, \qquad \omega_0 = \sqrt{k/m}. \tag{5.25}$$

For $\omega \neq \omega_0$, a particular solution is

$$\langle x\rangle_{\mathrm{p}}(t) = -\frac{qE_0/m}{\omega_0^2 - \omega^2}\cos\omega t. \tag{5.26}$$

The full solution includes the homogeneous oscillation fixed by both $\langle x\rangle(0)$ and $\langle p\rangle(0)$. Specifying only $\langle x\rangle(0)$ is not enough to determine a unique solution. If $v_0 = \langle p\rangle(0)/m$, then for $\omega \neq \omega_0$,

$$\begin{aligned}\langle x\rangle(t) = {}& \left[x_0 + \frac{qE_0/m}{\omega_0^2 - \omega^2}\right]\cos\omega_0 t + \frac{v_0}{\omega_0}\sin\omega_0 t \\ & - \frac{qE_0/m}{\omega_0^2 - \omega^2}\cos\omega t.\end{aligned} \tag{5.27}$$

At resonance, $\omega = \omega_0$, a particular solution is

$$\langle x\rangle_{\mathrm{p}}(t) = -\frac{qE_0}{2m\omega_0}\,t\sin\omega_0 t, \tag{5.28}$$

again supplemented by the homogeneous solution.

5.6 Rate of change of the energy

Applying Ehrenfest's theorem to the Hamiltonian itself,

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle H\rangle = \left\langle \frac{\partial H}{\partial t}\right\rangle, \tag{5.29}$$

since $[H, H] = 0$. For the driven oscillator above,

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle H\rangle = -qE_0\omega\sin\omega t\,\langle x\rangle. \tag{5.30}$$

This is the power supplied by the explicitly time-dependent external field.

5.7 Constants of motion

An observable A is conserved if its expectation value is time-independent for all states. A sufficient operator condition is

$$\frac{\partial A}{\partial t} = 0, \qquad [A, H] = 0. \tag{5.31}$$

Then

$$\frac{\mathrm{d}\langle A\rangle}{\mathrm{d}t} = 0. \tag{5.32}$$

If A commutes with H, transition matrix elements between nondegenerate energy eigenstates vanish:

$$(E_m - E_n)\langle m|A|n\rangle = 0. \tag{5.33}$$

Hence A is block diagonal in energy eigenspaces.

5.8 Schrödinger picture

In the Schrödinger picture, states carry the time dependence and operators are fixed unless they have explicit time dependence:

$$|\psi_S(t)\rangle = U(t,t_0)\,|\psi_S(t_0)\rangle\,. \tag{5.34}$$

An observable is represented by $A_S(t)$, with only explicit time dependence included in A_S.

5.9 Heisenberg picture

Choose t_0 as reference. The Heisenberg state is constant,

$$|\psi_H\rangle = |\psi_S(t_0)\rangle\,, \tag{5.35}$$

and the operator is

$$A_H(t) = U^\dagger(t,t_0)A_S(t)U(t,t_0). \tag{5.36}$$

Its equation of motion is

$$\boxed{\frac{\mathrm{d}A_H}{\mathrm{d}t} = \left(\frac{\partial A}{\partial t}\right)_H + \frac{\mathrm{i}}{\hbar}\,[H_H, A_H]}. \tag{5.37}$$

For a time-independent Hamiltonian,

$$H_H = H_S = H. \tag{5.38}$$

Expectation values are picture-independent:

$$\langle\psi_S(t)|A_S|\psi_S(t)\rangle = \langle\psi_H|A_H(t)|\psi_H\rangle\,. \tag{5.39}$$

5.10 Interaction picture

If

$$H = H_0 + V(t), \tag{5.40}$$

define

$$U_0(t,t_0) = \exp\left[-\frac{\mathrm{i}H_0(t-t_0)}{\hbar}\right] \tag{5.41}$$

when H_0 is time-independent. The interaction-picture state and operator are

$$|\psi_I(t)\rangle = U_0^\dagger(t,t_0)\,|\psi_S(t)\rangle\,, \qquad A_I(t) = U_0^\dagger A_S U_0. \tag{5.42}$$

The state evolves under

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\,|\psi_I(t)\rangle = V_I(t)\,|\psi_I(t)\rangle\,, \tag{5.43}$$

where

$$V_I(t) = U_0^\dagger V(t)U_0. \tag{5.44}$$

This picture is the natural starting point for time-dependent perturbation theory.

Chapter 6

Density Operators, Statistical Mixtures, and Composite Systems

6.1 Pure-state density operator

For a normalized pure state $|\psi\rangle$, define

$$\rho = |\psi\rangle\langle\psi| . \tag{6.1}$$

Then

$$\rho^\dagger = \rho, \qquad \rho^2 = \rho, \qquad \operatorname{Tr}\rho = 1. \tag{6.2}$$

For any state $|\phi\rangle$,

$$\langle\phi|\rho|\phi\rangle = |\langle\phi|\psi\rangle|^2 \geq 0, \tag{6.3}$$

so ρ is positive semidefinite.

Expectation values may be written as

$$\boxed{\langle A\rangle = \operatorname{Tr}(\rho A)}. \tag{6.4}$$

Indeed, in any orthonormal basis $\{|u_n\rangle\}$,

$$\operatorname{Tr}(\rho A) = \sum_n \langle u_n|\psi\rangle \langle\psi|A|u_n\rangle \tag{6.5}$$

$$= \langle\psi|A|\psi\rangle . \tag{6.6}$$

6.2 Statistical mixtures

Suppose an ensemble contains normalized pure states $|\psi_i\rangle$ with classical probabilities p_i satisfying

$$p_i \geq 0, \qquad \sum_i p_i = 1. \tag{6.7}$$

The density operator is

$$\boxed{\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|}. \tag{6.8}$$

It is Hermitian, positive semidefinite, and has unit trace. In general,

$$\rho^2 \neq \rho. \tag{6.9}$$

The spectral decomposition of any density operator is

$$\rho = \sum_n \lambda_n |n\rangle\langle n| \,, \tag{6.10}$$

with

$$\lambda_n \geq 0, \qquad \sum_n \lambda_n = 1. \tag{6.11}$$

The eigenvalues may therefore be interpreted as probabilities in the eigenbasis of ρ.

6.3 Purity

The purity is

$$\gamma = \mathrm{Tr}(\rho^2). \tag{6.12}$$

For a finite-dimensional system,

$$\frac{1}{d} \leq \gamma \leq 1. \tag{6.13}$$

A density operator describes a pure state iff

$$\boxed{\mathrm{Tr}(\rho^2) = 1} \tag{6.14}$$

or equivalently $\rho^2 = \rho$. A genuinely mixed state has

$$\mathrm{Tr}(\rho^2) < 1. \tag{6.15}$$

The maximally mixed state in dimension d is

$$\rho_{\mathrm{mm}} = \frac{I}{d}, \tag{6.16}$$

with purity $1/d$.

6.4 Populations and coherences

In a chosen basis $\{|n\rangle\}$,

$$\rho_{mn} = \langle m|\rho|n\rangle \,. \tag{6.17}$$

The diagonal entries ρ_{nn} are populations. Off-diagonal entries are coherences relative to that basis. Hermiticity gives

$$\rho_{mn} = \rho^*_{nm}. \tag{6.18}$$

Positivity implies

$$|\rho_{mn}|^2 \leq \rho_{mm}\rho_{nn}. \tag{6.19}$$

Whether an entry is called a population or coherence is basis-dependent, but the eigenvalues, purity, and entropy are basis-independent.

6.5 Unpolarized two-level system

For a two-level system, the equal incoherent mixture of two orthogonal basis states is

$$\rho = \frac{1}{2}\left|+\right\rangle\left\langle+\right| + \frac{1}{2}\left|-\right\rangle\left\langle-\right| = \frac{1}{2}I. \tag{6.20}$$

No pure state vector can reproduce this density matrix. A pure superposition

$$\frac{1}{\sqrt{2}}(\left|+\right\rangle + \mathrm{e}^{\mathrm{i}\varphi}\left|-\right\rangle) \tag{6.21}$$

has off-diagonal coherences and is therefore physically distinguishable from the unpolarized mixture by suitable measurements.

6.6 Time evolution of the density operator

For a closed system,

$$\rho(t) = U(t, t_0)\rho(t_0)U^\dagger(t, t_0). \tag{6.22}$$

Differentiating gives the von Neumann equation

$$\boxed{\mathrm{i}\hbar\frac{\mathrm{d}\rho}{\mathrm{d}t} = [H, \rho]}. \tag{6.23}$$

For a time-independent Hamiltonian, if $\rho(0)$ is diagonal in the energy basis then

$$[H, \rho] = 0 \tag{6.24}$$

and the density operator is stationary. More generally, in the energy basis,

$$\rho_{mn}(t) = \rho_{mn}(0)\mathrm{e}^{-\mathrm{i}(E_m - E_n)t/\hbar}. \tag{6.25}$$

Populations are constant under isolated unitary evolution, while energy-basis coherences acquire phases.

6.7 Thermal equilibrium

In the canonical ensemble at temperature T,

$$\boxed{\rho_\beta = \frac{\mathrm{e}^{-\beta H}}{Z}}, \qquad \beta = \frac{1}{k_B T}, \qquad Z = \mathrm{Tr}\,\mathrm{e}^{-\beta H}. \tag{6.26}$$

Since ρ_β is a function of H,

$$[H, \rho_\beta] = 0, \tag{6.27}$$

so it is stationary for an isolated system. In the energy basis,

$$\rho_\beta = \frac{1}{Z}\sum_n \mathrm{e}^{-\beta E_n}\left|n\right\rangle\left\langle n\right|. \tag{6.28}$$

The thermal expectation value is

$$\langle A\rangle_\beta = \mathrm{Tr}(\rho_\beta A). \tag{6.29}$$

Useful thermodynamic identities include

$$\langle H\rangle = -\frac{\partial \ln Z}{\partial\beta}, \qquad (\Delta H)^2 = \frac{\partial^2 \ln Z}{\partial\beta^2}. \tag{6.30}$$

6.8 Composite systems and reduced density matrices

Let the total Hilbert space be

$$\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B. \tag{6.31}$$

A general pure state is

$$|\Psi\rangle = \sum_{ij} c_{ij} |i\rangle_A \otimes |j\rangle_B \,. \tag{6.32}$$

The total density operator is

$$\rho_{AB} = |\Psi\rangle\langle\Psi| \,. \tag{6.33}$$

If only subsystem A is accessible, its reduced density operator is obtained by tracing out B:

$$\boxed{\rho_A = \mathrm{Tr}_B\, \rho_{AB}}. \tag{6.34}$$

In an orthonormal basis $\{|j\rangle_B\}$,

$$\rho_A = \sum_j {}_B\langle j| \rho_{AB} |j\rangle_B \,. \tag{6.35}$$

Similarly,

$$\rho_B = \mathrm{Tr}_A\, \rho_{AB}. \tag{6.36}$$

For any observable A acting only on subsystem A,

$$\mathrm{Tr}_{AB}\, [\rho_{AB}(A \otimes I_B)] = \mathrm{Tr}_A(\rho_A A). \tag{6.37}$$

6.9 Product states and entanglement

If

$$|\Psi\rangle = |\psi\rangle_A \otimes |\phi\rangle_B \,, \tag{6.38}$$

then

$$\rho_A = |\psi\rangle\langle\psi| \,, \tag{6.39}$$

which is pure. If a bipartite pure state is entangled, its reduced density matrix is mixed. For example, the Bell state

$$\left|\Phi^+\right\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) \tag{6.40}$$

has

$$\rho_A = \rho_B = \frac{1}{2} I. \tag{6.41}$$

The total state is pure while each subsystem separately is maximally mixed.

6.10 Schmidt decomposition

Any pure bipartite state admits a Schmidt decomposition

$$|\Psi\rangle = \sum_{k=1}^{r} \sqrt{\lambda_k}\, |u_k\rangle_A |v_k\rangle_B \,, \tag{6.42}$$

where

$$\lambda_k \geq 0, \qquad \sum_k \lambda_k = 1. \tag{6.43}$$

The reduced density operators have the same nonzero eigenvalues:

$$\rho_A = \sum_k \lambda_k \, |u_k\rangle\langle u_k| \,, \qquad \rho_B = \sum_k \lambda_k \, |v_k\rangle\langle v_k| \,. \tag{6.44}$$

The state is separable iff the Schmidt rank is one.

Chapter 7

The One-Dimensional Harmonic Oscillator

7.1 Hamiltonian and natural scales

The harmonic-oscillator Hamiltonian is

$$H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2, \tag{7.1}$$

where

$$\omega = \sqrt{k/m}. \tag{7.2}$$

A natural length scale is

$$x_0 = \sqrt{\frac{\hbar}{m\omega}}, \tag{7.3}$$

and it is convenient to define dimensionless operators

$$Q = \sqrt{\frac{m\omega}{\hbar}}\, x, \qquad P = \frac{p}{\sqrt{m\hbar\omega}}, \tag{7.4}$$

which obey

$$[Q, P] = \mathrm{i}. \tag{7.5}$$

Then

$$H = \frac{\hbar\omega}{2}(P^2 + Q^2). \tag{7.6}$$

7.2 Creation and annihilation operators

Define

$$a = \frac{1}{\sqrt{2}}(Q + \mathrm{i}P), \qquad a^\dagger = \frac{1}{\sqrt{2}}(Q - \mathrm{i}P). \tag{7.7}$$

Equivalently,

$$a = \sqrt{\frac{m\omega}{2\hbar}} x + \frac{\mathrm{i}}{\sqrt{2m\hbar\omega}} p, \tag{7.8}$$

$$a^\dagger = \sqrt{\frac{m\omega}{2\hbar}} x - \frac{\mathrm{i}}{\sqrt{2m\hbar\omega}} p. \tag{7.9}$$

Using $[x, p] = \mathrm{i}\hbar$,

$$\boxed{\left[a, a^\dagger\right] = 1}. \tag{7.10}$$

Define the number operator

$$N = a^\dagger a. \tag{7.11}$$

Then

$$H = \hbar\omega\left(N + \frac{1}{2}\right), \tag{7.12}$$

and

$$[N, a] = -a, \qquad \left[N, a^\dagger\right] = a^\dagger. \tag{7.13}$$

7.3 Spectrum

Let

$$N\left|n\right\rangle = n\left|n\right\rangle. \tag{7.14}$$

Since

$$\langle\psi|N|\psi\rangle = \|a\left|\psi\right\rangle\|^2 \geq 0, \tag{7.15}$$

the eigenvalues of N are nonnegative. Laddering gives

$$a\left|n\right\rangle = \sqrt{n}\left|n-1\right\rangle, \qquad a^\dagger\left|n\right\rangle = \sqrt{n+1}\left|n+1\right\rangle. \tag{7.16}$$

The lowering process must terminate at a state $\left|0\right\rangle$ satisfying

$$a\left|0\right\rangle = 0. \tag{7.17}$$

Thus

$$\boxed{n = 0, 1, 2, \ldots} \tag{7.18}$$

and

$$\boxed{E_n = \hbar\omega\left(n + \frac{1}{2}\right)}. \tag{7.19}$$

Normalized excited states are

$$\left|n\right\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}}\left|0\right\rangle. \tag{7.20}$$

7.4 Position-space ground state

The ground-state condition

$$a\psi_0(x) = 0 \tag{7.21}$$

becomes

$$\left(\sqrt{\frac{m\omega}{2\hbar}}x + \sqrt{\frac{\hbar}{2m\omega}}\frac{\mathrm{d}}{\mathrm{d}x}\right)\psi_0(x) = 0. \tag{7.22}$$

Hence

$$\frac{\mathrm{d}\psi_0}{\mathrm{d}x} = -\frac{m\omega}{\hbar}x\psi_0, \tag{7.23}$$

and therefore

$$\boxed{\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{m\omega x^2}{2\hbar}\right)}. \tag{7.24}$$

7.5 Excited-state wave functions

The normalized energy eigenfunctions are

$$\boxed{\psi_n(x) = \frac{1}{\sqrt{2^n n!}} \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} H_n(\xi) e^{-\xi^2/2}}, \tag{7.25}$$

where

$$\xi = \sqrt{\frac{m\omega}{\hbar}} x \tag{7.26}$$

and H_n is the Hermite polynomial. The parity is

$$\psi_n(-x) = (-1)^n \psi_n(x). \tag{7.27}$$

7.6 Position and momentum in ladder form

Inverting the definitions,

$$x = \sqrt{\frac{\hbar}{2m\omega}} (a + a^\dagger), \tag{7.28}$$

$$p = -i\sqrt{\frac{m\hbar\omega}{2}} (a - a^\dagger). \tag{7.29}$$

The basic matrix elements are

$$\langle m|x|n\rangle = \sqrt{\frac{\hbar}{2m\omega}} \left(\sqrt{n}\,\delta_{m,n-1} + \sqrt{n+1}\,\delta_{m,n+1}\right), \tag{7.30}$$

and

$$\langle m|p|n\rangle = -i\sqrt{\frac{m\hbar\omega}{2}} \left(\sqrt{n}\,\delta_{m,n-1} - \sqrt{n+1}\,\delta_{m,n+1}\right). \tag{7.31}$$

Thus x and p connect only states with $\Delta n = \pm 1$.

7.7 Quadratic moments

Using

$$x^2 = \frac{\hbar}{2m\omega} \left(a^2 + a^{\dagger 2} + 2N + 1\right), \tag{7.32}$$

we find

$$\boxed{\left\langle n \middle| x^2 \middle| n \right\rangle = \frac{\hbar}{m\omega} \left(n + \frac{1}{2}\right)}. \tag{7.33}$$

Similarly,

$$\boxed{\left\langle n \middle| p^2 \middle| n \right\rangle = m\hbar\omega \left(n + \frac{1}{2}\right)}. \tag{7.34}$$

Since $\langle x\rangle = \langle p\rangle = 0$ in number states,

$$\Delta x = \sqrt{\frac{\hbar}{m\omega} \left(n + \frac{1}{2}\right)}, \tag{7.35}$$

$$\Delta p = \sqrt{m\hbar\omega\left(n+\frac{1}{2}\right)}. \tag{7.36}$$

Hence

$$\Delta x \Delta p = \hbar\left(n+\frac{1}{2}\right). \tag{7.37}$$

The ground state saturates the Heisenberg bound:

$$\Delta x \Delta p = \frac{\hbar}{2}. \tag{7.38}$$

7.8 Fourth moment

A useful result, appearing in the course problem material, is

$$\boxed{\left\langle n\middle|x^4\middle|n\right\rangle = \frac{3\hbar^2}{4m^2\omega^2}\left(2n^2+2n+1\right)}. \tag{7.39}$$

For a quartic perturbation

$$H = H_0 + \lambda x^4, \tag{7.40}$$

the first-order perturbative shift would be

$$E_n^{(1)} = \lambda\left\langle n\middle|x^4\middle|n\right\rangle, \tag{7.41}$$

although perturbation theory itself lies beyond the main handwritten notebook sequence.

7.9 Two coupled oscillators: center-of-mass and relative modes

A worked example in the accompanying problem material considers two oscillators with masses m_1, m_2, a common trap frequency ω, and coupling

$$H = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + \frac{1}{2}m_1\omega^2 x_1^2 + \frac{1}{2}m_2\omega^2 x_2^2 + \frac{1}{2}K(x_1-x_2)^2. \tag{7.42}$$

Define

$$X = \frac{m_1x_1+m_2x_2}{M}, \qquad x = x_1 - x_2, \tag{7.43}$$

$$P = p_1 + p_2, \qquad p = \frac{m_2p_1 - m_1p_2}{M}, \tag{7.44}$$

where

$$M = m_1 + m_2, \qquad \mu = \frac{m_1m_2}{M}. \tag{7.45}$$

These are canonical pairs,

$$[X,P] = [x,p] = \mathrm{i}\hbar, \qquad [X,p] = [x,P] = 0. \tag{7.46}$$

The Hamiltonian separates exactly:

$$H = \underbrace{\frac{P^2}{2M} + \frac{1}{2}M\omega^2X^2}_{H_{\mathrm{CM}}} + \underbrace{\frac{p^2}{2\mu} + \frac{1}{2}\mu\Omega^2x^2}_{H_{\mathrm{rel}}}, \tag{7.47}$$

with

$$\boxed{\Omega^2 = \omega^2 + \frac{K}{\mu}}. \tag{7.48}$$

Hence

$$\boxed{E_{n_{\mathrm{CM}},n_{\mathrm{rel}}} = \hbar\omega\left(n_{\mathrm{CM}} + \frac{1}{2}\right) + \hbar\Omega\left(n_{\mathrm{rel}} + \frac{1}{2}\right)}. \tag{7.49}$$

This derivation also illustrates the same center-of-mass/reduced-mass transformation used later for the two-body central-force problem.

7.10 Heisenberg-picture oscillator

For the time-independent harmonic oscillator,

$$\frac{\mathrm{d}a_H}{\mathrm{d}t} = \frac{\mathrm{i}}{\hbar}[H, a_H] = -\mathrm{i}\omega a_H, \tag{7.50}$$

so

$$a_H(t) = a\mathrm{e}^{-\mathrm{i}\omega t}, \qquad a_H^\dagger(t) = a^\dagger \mathrm{e}^{\mathrm{i}\omega t}. \tag{7.51}$$

Therefore

$$x_H(t) = x(0)\cos\omega t + \frac{p(0)}{m\omega}\sin\omega t, \tag{7.52}$$

which has the same form as the classical solution.

7.11 Thermal harmonic oscillator

For

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right), \tag{7.53}$$

the canonical partition function is

$$\begin{aligned} Z &= \sum_{n=0}^{\infty} \mathrm{e}^{-\beta\hbar\omega(n+1/2)} && (7.54)\\ &= \frac{\mathrm{e}^{-\beta\hbar\omega/2}}{1-\mathrm{e}^{-\beta\hbar\omega}} && (7.55)\\ &= \frac{1}{2\sinh(\beta\hbar\omega/2)}. && (7.56) \end{aligned}$$

The mean energy is

$$\boxed{\langle H\rangle = -\frac{\partial \ln Z}{\partial\beta} = \frac{\hbar\omega}{2}\coth\left(\frac{\beta\hbar\omega}{2}\right)}. \tag{7.57}$$

Equivalently,

$$\langle H\rangle = \frac{\hbar\omega}{2} + \frac{\hbar\omega}{\mathrm{e}^{\beta\hbar\omega}-1}. \tag{7.58}$$

The first term is the zero-point energy and the second is the thermal Bose factor.

7.12 Thermal position distribution

The thermal density operator is

$$\rho_\beta = \frac{e^{-\beta H}}{Z}. \tag{7.59}$$

The position probability density is

$$P_\beta(x) = \langle x|\rho_\beta|x\rangle\,. \tag{7.60}$$

For the harmonic oscillator it is exactly Gaussian:

$$\boxed{P_\beta(x) = \sqrt{\frac{m\omega}{\pi\hbar}\tanh\left(\frac{\beta\hbar\omega}{2}\right)}\exp\left[-\frac{m\omega x^2}{\hbar}\tanh\left(\frac{\beta\hbar\omega}{2}\right)\right]}. \tag{7.61}$$

Its variance is

$$\boxed{\langle x^2\rangle_\beta = \frac{\hbar}{2m\omega}\coth\left(\frac{\beta\hbar\omega}{2}\right)}. \tag{7.62}$$

It is sometimes convenient to write

$$P_\beta(x) = \frac{1}{\sqrt{\pi}\,\xi_T}e^{-x^2/\xi_T^2}, \tag{7.63}$$

where

$$\xi_T^2 = \frac{\hbar}{m\omega}\coth\left(\frac{\beta\hbar\omega}{2}\right) = 2\langle x^2\rangle_\beta. \tag{7.64}$$

At $T \to 0$, this reduces to the ground-state probability distribution; at high temperature,

$$\langle x^2\rangle_\beta \longrightarrow \frac{k_B T}{m\omega^2}, \tag{7.65}$$

in agreement with classical equipartition.

Part II

Angular Momentum and Rotations

Chapter 8

General Theory of Angular Momentum

8.1 Angular-momentum algebra

An angular-momentum operator $\boldsymbol{J} = (J_x, J_y, J_z)$ is defined by the commutation relations

$$\boxed{[J_i, J_j] = \mathrm{i}\hbar\epsilon_{ijk}J_k}. \tag{8.1}$$

Thus

$$[J_x, J_y] = \mathrm{i}\hbar J_z, \tag{8.2}$$
$$[J_y, J_z] = \mathrm{i}\hbar J_x, \tag{8.3}$$
$$[J_z, J_x] = \mathrm{i}\hbar J_y. \tag{8.4}$$

Define

$$J^2 = J_x^2 + J_y^2 + J_z^2. \tag{8.5}$$

A direct calculation gives

$$\boxed{\left[J^2, J_i\right] = 0} \tag{8.6}$$

for $i = x, y, z$. Hence J^2 and any one Cartesian component, conventionally J_z, can be diagonalized simultaneously.

8.2 Ladder operators

Define

$$J_\pm = J_x \pm \mathrm{i}J_y. \tag{8.7}$$

Then

$$J_x = \frac{1}{2}(J_+ + J_-), \qquad J_y = \frac{1}{2\mathrm{i}}(J_+ - J_-). \tag{8.8}$$

The commutators are

$$\boxed{[J_z, J_\pm] = \pm\hbar J_\pm}, \tag{8.9}$$

$$\boxed{[J_+, J_-] = 2\hbar J_z}, \tag{8.10}$$

and

$$\left[J^2, J_\pm\right] = 0. \tag{8.11}$$

Useful identities are

$$J_-J_+ = J^2 - J_z^2 - \hbar J_z, \tag{8.12}$$
$$J_+J_- = J^2 - J_z^2 + \hbar J_z. \tag{8.13}$$

8.3 Simultaneous eigenstates of J^2 and J_z

Choose states $|j,m\rangle$ satisfying

$$J^2 |j,m\rangle = \hbar^2 j(j+1) |j,m\rangle, \tag{8.14}$$

$$J_z |j,m\rangle = \hbar m |j,m\rangle. \tag{8.15}$$

The labels are

$$j = 0, \frac{1}{2}, 1, \frac{3}{2}, \dots, \qquad m = -j, -j+1, \dots, j-1, j. \tag{8.16}$$

There are

$$\boxed{2j+1} \tag{8.17}$$

states in an irreducible j multiplet.

8.4 Derivation of the allowed m values

Since norms are nonnegative,

$$\|J_+ |j,m\rangle\|^2 = \langle j,m|J_-J_+|j,m\rangle \tag{8.18}$$
$$= \hbar^2 [j(j+1) - m(m+1)] \geq 0, \tag{8.19}$$

while

$$\|J_- |j,m\rangle\|^2 = \hbar^2 [j(j+1) - m(m-1)] \geq 0. \tag{8.20}$$

Repeated raising must terminate at a highest state $|j,j\rangle$ and repeated lowering at $|j,-j\rangle$. The step size is one, so $2j$ must be an integer, implying that j is integer or half-integer.

8.5 Normalized ladder action

Choosing the standard positive phase convention,

$$\boxed{J_+ |j,m\rangle = \hbar\sqrt{(j-m)(j+m+1)}\, |j,m+1\rangle}, \tag{8.21}$$

$$\boxed{J_- |j,m\rangle = \hbar\sqrt{(j+m)(j-m+1)}\, |j,m-1\rangle}. \tag{8.22}$$

The highest and lowest states obey

$$J_+ |j,j\rangle = 0, \qquad J_- |j,-j\rangle = 0. \tag{8.23}$$

8.6 Matrix representation in the $|j, m\rangle$ basis

Order the basis as

$$|j, j\rangle, |j, j-1\rangle, \ldots, |j, -j\rangle. \tag{8.24}$$

Then

$$J_z = \hbar \,\mathrm{diag}(j, j-1, \ldots, -j), \tag{8.25}$$

and J_+ has nonzero entries only immediately above or below the diagonal depending on the chosen basis ordering. Once $J_\pm$ are known,

$$J_x = \frac{1}{2}(J_+ + J_-), \qquad J_y = \frac{1}{2\mathrm{i}}(J_+ - J_-). \tag{8.26}$$

8.7 Example: $j = \frac{1}{2}$

In the basis $\{|+\rangle, |-\rangle\} = \{|1/2, 1/2\rangle, |1/2, -1/2\rangle\}$,

$$J_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \tag{8.27}$$

$$J_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \tag{8.28}$$

$$J_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{8.29}$$

Thus

$$J_i = \frac{\hbar}{2}\sigma_i, \tag{8.30}$$

where σ_i are the Pauli matrices.

8.8 Example: $j = 1$

In the ordered basis $\{|1, 1\rangle, |1, 0\rangle, |1, -1\rangle\}$,

$$J_z = \hbar\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \tag{8.31}$$

$$J_+ = \sqrt{2}\hbar\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}, \qquad J_- = \sqrt{2}\hbar\begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}. \tag{8.32}$$

Therefore

$$J_x = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \tag{8.33}$$

$$J_y = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & -\mathrm{i} & 0 \\ \mathrm{i} & 0 & -\mathrm{i} \\ 0 & \mathrm{i} & 0 \end{pmatrix}. \tag{8.34}$$

8.9 Angular momentum and uncertainty

In $|j, m\rangle$,

$$\langle J_x \rangle = \langle J_y \rangle = 0. \tag{8.35}$$

Using rotational symmetry around the z axis,

$$\langle J_x^2 \rangle = \langle J_y^2 \rangle = \frac{\hbar^2}{2} \left[j(j+1) - m^2 \right]. \tag{8.36}$$

Hence

$$\Delta J_x \Delta J_y = \frac{\hbar^2}{2} \left[j(j+1) - m^2 \right] \geq \frac{\hbar}{2} |\langle J_z \rangle| = \frac{\hbar^2}{2} |m|. \tag{8.37}$$

The Robertson lower bound is saturated only for extremal states $m = \pm j$.

8.10 Orbital angular momentum as an example

For a particle in three dimensions,

$$\boldsymbol{L} = \boldsymbol{r} \times \boldsymbol{p}. \tag{8.38}$$

Canonical commutation relations imply

$$[L_i, L_j] = \mathrm{i}\hbar \epsilon_{ijk} L_k, \tag{8.39}$$

so orbital angular momentum satisfies the abstract angular-momentum algebra. In addition,

$$[L_i, r_j] = \mathrm{i}\hbar \epsilon_{ijk} r_k, \qquad [L_i, p_j] = \mathrm{i}\hbar \epsilon_{ijk} p_k, \tag{8.40}$$

which expresses the fact that $\boldsymbol{r}$ and $\boldsymbol{p}$ transform as vectors under rotations.

Chapter 9

Addition of Angular Momenta and Clebsch–Gordan Coefficients

9.1 Total angular momentum of two subsystems

Let two independent angular momenta be $\boldsymbol{J}_1$ and $\boldsymbol{J}_2$, acting on

$$\mathcal{H} = \mathcal{H}_{j_1} \otimes \mathcal{H}_{j_2}. \tag{9.1}$$

Since they act on different tensor factors,

$$[J_{1i}, J_{2j}] = 0. \tag{9.2}$$

Define total angular momentum

$$\boxed{\boldsymbol{J} = \boldsymbol{J}_1 + \boldsymbol{J}_2}. \tag{9.3}$$

It also satisfies

$$[J_i, J_j] = \mathrm{i}\hbar\epsilon_{ijk} J_k. \tag{9.4}$$

Moreover,

$$J^2 = J_1^2 + J_2^2 + 2\boldsymbol{J}_1 \cdot \boldsymbol{J}_2. \tag{9.5}$$

9.2 Uncoupled and coupled bases

The uncoupled basis diagonalizes

$$\{J_1^2, J_2^2, J_{1z}, J_{2z}\}: \tag{9.6}$$

$$|j_1 m_1; j_2 m_2\rangle \equiv |j_1, m_1\rangle \otimes |j_2, m_2\rangle. \tag{9.7}$$

The coupled basis diagonalizes

$$\{J_1^2, J_2^2, J^2, J_z\}: \tag{9.8}$$

$$|j_1 j_2; JM\rangle. \tag{9.9}$$

Because

$$J_z = J_{1z} + J_{2z}, \tag{9.10}$$

a nonzero overlap requires

$$\boxed{M = m_1 + m_2}. \tag{9.11}$$

9.3 Allowed values of J

The tensor-product representation decomposes as

$$\boxed{j_1 \otimes j_2 = \bigoplus_{J=|j_1-j_2|}^{j_1+j_2} J}. \tag{9.12}$$

Thus

$$J = |j_1 - j_2|, |j_1 - j_2| + 1, \ldots, j_1 + j_2. \tag{9.13}$$

A dimension check gives

$$(2j_1 + 1)(2j_2 + 1) = \sum_{J=|j_1-j_2|}^{j_1+j_2} (2J + 1). \tag{9.14}$$

9.4 Clebsch–Gordan coefficients

The change of basis is

$$\boxed{|j_1 j_2; JM\rangle = \sum_{m_1,m_2} C^{JM}_{j_1 m_1, j_2 m_2} \, |j_1 m_1; j_2 m_2\rangle}, \tag{9.15}$$

where

$$C^{JM}_{j_1 m_1, j_2 m_2} = \langle j_1 m_1; j_2 m_2 | j_1 j_2; JM\rangle \,. \tag{9.16}$$

The coefficient vanishes unless

$$M = m_1 + m_2. \tag{9.17}$$

With the standard Condon–Shortley phase convention the coefficients may be chosen real.

The inverse transformation is

$$|j_1 m_1; j_2 m_2\rangle = \sum_{J,M} C^{JM}_{j_1 m_1, j_2 m_2} \, |j_1 j_2; JM\rangle \,. \tag{9.18}$$

9.5 Orthogonality and completeness of CG coefficients

Unitarity of the basis change implies

$$\sum_{m_1,m_2} C^{JM}_{j_1 m_1, j_2 m_2} C^{J'M'}_{j_1 m_1, j_2 m_2} = \delta_{JJ'} \delta_{MM'}, \tag{9.19}$$

and

$$\sum_{J,M} C^{JM}_{j_1 m_1, j_2 m_2} C^{JM}_{j_1 m_1', j_2 m_2'} = \delta_{m_1 m_1'} \delta_{m_2 m_2'}. \tag{9.20}$$

9.6 Highest-weight construction

The unique state with maximum total magnetic quantum number

$$M_{\max} = j_1 + j_2 \tag{9.21}$$

is

$$|J = j_1 + j_2, M = J\rangle = |j_1, j_1; j_2, j_2\rangle \,. \tag{9.22}$$

The rest of that multiplet follows by applying

$$J_- = J_{1-} + J_{2-}. \tag{9.23}$$

After constructing the $J = j_1 + j_2$ multiplet, the next-highest M subspace contains one vector orthogonal to the already constructed state; that vector seeds the $J = j_1 + j_2 - 1$ multiplet. Continuing recursively constructs the entire decomposition.

9.7 Recursion relation

Apply $J_\pm = J_{1\pm} + J_{2\pm}$ to a coupled state. Comparing coefficients gives

$$\sqrt{(J \mp M)(J \pm M + 1)}C^{J,M\pm1}_{j_1m_1,j_2m_2} \tag{9.24}$$

$$= \sqrt{(j_1 \pm m_1)(j_1 \mp m_1 + 1)}C^{JM}_{j_1,m_1\mp1;j_2,m_2} \tag{9.25}$$

$$+ \sqrt{(j_2 \pm m_2)(j_2 \mp m_2 + 1)}C^{JM}_{j_1,m_1;j_2,m_2\mp1}. \tag{9.26}$$

For the upper signs this is the raising recursion and for the lower signs it is the lowering recursion. Each term automatically respects $M = m_1 + m_2$ in the coefficient on its own side of the relation.

9.8 Exchange symmetry

With the Condon–Shortley convention,

$$\boxed{C^{JM}_{j_2m_2,j_1m_1} = (-1)^{j_1+j_2-J}C^{JM}_{j_1m_1,j_2m_2}}. \tag{9.27}$$

Another useful symmetry is

$$C^{J,-M}_{j_1,-m_1,j_2,-m_2} = (-1)^{j_1+j_2-J}C^{JM}_{j_1m_1,j_2m_2}. \tag{9.28}$$

These phase relations are convention-dependent in appearance, so a phase convention must be stated whenever signs matter.

9.9 Example: $\frac{1}{2} \otimes \frac{1}{2}$

The decomposition is

$$\frac{1}{2} \otimes \frac{1}{2} = 1 \oplus 0. \tag{9.29}$$

The triplet states are

$$|1, 1\rangle = |{+}{+}\rangle \,, \tag{9.30}$$

$$|1, 0\rangle = \frac{1}{\sqrt{2}}(|{+}{-}\rangle + |{-}{+}\rangle), \tag{9.31}$$

$$|1, -1\rangle = |{-}{-}\rangle \,, \tag{9.32}$$

and the singlet is

$$\boxed{|0, 0\rangle = \frac{1}{\sqrt{2}}(|{+}{-}\rangle - |{-}{+}\rangle)}. \tag{9.33}$$

The triplet is symmetric under particle exchange while the singlet is antisymmetric in spin labels.

9.10 Example: $1 \otimes 1$

The decomposition is

$$1 \otimes 1 = 2 \oplus 1 \oplus 0. \tag{9.34}$$

The $J = 2$ multiplet begins with

$$|2, 2\rangle = |1, 1; 1, 1\rangle . \tag{9.35}$$

Lowering once gives

$$|2, 1\rangle = \frac{1}{\sqrt{2}} \left(|1, 1; 1, 0\rangle + |1, 0; 1, 1\rangle\right). \tag{9.36}$$

The orthogonal state at $M = 1$ is

$$|1, 1\rangle = \frac{1}{\sqrt{2}} \left(|1, 1; 1, 0\rangle - |1, 0; 1, 1\rangle\right). \tag{9.37}$$

At $M = 0$, one obtains

$$|2, 0\rangle = \frac{1}{\sqrt{6}} \left(|1, 1; 1, -1\rangle + 2\,|1, 0; 1, 0\rangle + |1, -1; 1, 1\rangle\right), \tag{9.38}$$

$$|1, 0\rangle = \frac{1}{\sqrt{2}} \left(|1, 1; 1, -1\rangle - |1, -1; 1, 1\rangle\right), \tag{9.39}$$

$$\boxed{|0, 0\rangle = \frac{1}{\sqrt{3}} \left(|1, 1; 1, -1\rangle - |1, 0; 1, 0\rangle + |1, -1; 1, 1\rangle\right)}. \tag{9.40}$$

The remaining states follow by lowering or by the symmetry relations above.

9.11 Scalar product of two angular momenta

Since

$$J^2 = J_1^2 + J_2^2 + 2\boldsymbol{J}_1 \cdot \boldsymbol{J}_2, \tag{9.41}$$

we have

$$\boxed{\boldsymbol{J}_1 \cdot \boldsymbol{J}_2 = \frac{1}{2}\left(J^2 - J_1^2 - J_2^2\right)}. \tag{9.42}$$

Thus in the coupled basis,

$$\boldsymbol{J}_1 \cdot \boldsymbol{J}_2\, |j_1 j_2; JM\rangle = \frac{\hbar^2}{2}\left[J(J+1) - j_1(j_1+1) - j_2(j_2+1)\right] |j_1 j_2; JM\rangle . \tag{9.43}$$

This identity is central to spin–spin and spin–orbit interactions.

9.12 Spherical tensor operators

An irreducible spherical tensor operator of rank k consists of components

$$T_q^{(k)}, \qquad q = -k, -k+1, \ldots, k, \tag{9.44}$$

that transform under rotations like an angular-momentum-k multiplet. Their commutators with angular momentum are

$$\left[J_z, T_q^{(k)}\right] = \hbar q T_q^{(k)}, \tag{9.45}$$

$$\left[J_\pm, T_q^{(k)}\right] = \hbar\sqrt{(k \mp q)(k \pm q + 1)}\, T_{q\pm1}^{(k)}. \tag{9.46}$$

A scalar operator has $k = 0$; an ordinary vector operator corresponds to $k = 1$.

9.13 Wigner–Eckart theorem

The Wigner–Eckart theorem separates angular dependence from dynamical information. With one common convention,

$$\boxed{\left\langle j'm' \middle| T_q^{(k)} \middle| jm \right\rangle = \frac{\left\langle j' \middle| T^{(k)} \middle| j \right\rangle_{\text{red}}}{\sqrt{2j'+1}} C_{jm,kq}^{j'm'}}. \tag{9.47}$$

The reduced matrix element is independent of m, m', and q. Different textbooks absorb factors such as $\sqrt{2j'+1}$ and phase signs into the definition of the reduced matrix element; the physical content is unchanged.

Selection rules follow immediately:

$$m' = m + q, \tag{9.48}$$

and

$$|j - k| \leq j' \leq j + k. \tag{9.49}$$

For a vector operator ($k = 1$),

$$\Delta j = 0, \pm 1 \tag{9.50}$$

subject to the triangle conditions, and

$$\Delta m = 0, \pm 1. \tag{9.51}$$

Additional restrictions, such as parity, must be imposed separately.

Chapter 10

Vector Operators, Spin, and Two-Level Systems

10.1 Vector operators

A vector operator $\boldsymbol{V} = (V_x, V_y, V_z)$ transforms under rotations in the same way as an ordinary vector. Infinitesimally, this is equivalent to

$$\boxed{[J_i, V_j] = \mathrm{i}\hbar\epsilon_{ijk}V_k}. \tag{10.1}$$

For a finite rotation R represented by

$$U(R) = \exp\left(-\frac{\mathrm{i}}{\hbar}\theta\hat{\boldsymbol{n}}\cdot\boldsymbol{J}\right), \tag{10.2}$$

the operator transformation appropriate to an actively rotated state is

$$\boxed{U^\dagger(R)V_iU(R) = \sum_j R_{ij}V_j}. \tag{10.3}$$

Equivalently, $U(R)V_iU^\dagger(R) = \sum_j (R^{-1})_{ij}V_j$.

Examples include $\boldsymbol{r}$, $\boldsymbol{p}$, $\boldsymbol{L}$, and spin $\boldsymbol{S}$. A cross product of two commuting vector operators is also a vector; more generally operator ordering must be handled carefully.

10.2 Parity of vectors and pseudovectors

Under parity,

$$\boldsymbol{r} \to -\boldsymbol{r}, \qquad \boldsymbol{p} \to -\boldsymbol{p}. \tag{10.4}$$

Thus ordinary polar vectors are parity-odd. Angular momentum

$$\boldsymbol{L} = \boldsymbol{r}\times\boldsymbol{p} \tag{10.5}$$

is parity-even and is therefore an axial vector or pseudovector. Spin is also an axial vector.

10.3 Projection theorem for vector operators

Within a fixed irreducible j subspace, a vector operator has matrix elements proportional to those of $\boldsymbol{J}$. For diagonal matrix elements in j, one convenient form is

$$\boxed{P_j \boldsymbol{V} P_j = \frac{P_j(\boldsymbol{J} \cdot \boldsymbol{V})P_j}{\hbar^2 j(j+1)} \boldsymbol{J}}, \tag{10.6}$$

provided $j \neq 0$ and $\boldsymbol{J} \cdot \boldsymbol{V}$ acts as a scalar within the relevant irreducible sector. Consequently, in $|j, m\rangle$,

$$\langle V_z \rangle = \frac{m}{\hbar j(j+1)} \langle \boldsymbol{J} \cdot \boldsymbol{V} \rangle . \tag{10.7}$$

This is a special case of the Wigner–Eckart theorem.

10.4 Intrinsic spin

Spin is an intrinsic angular momentum. Its operators obey

$$[S_i, S_j] = \mathrm{i}\hbar\epsilon_{ijk} S_k. \tag{10.8}$$

Spin eigenstates satisfy

$$S^2 |s, m_s\rangle = \hbar^2 s(s+1) |s, m_s\rangle , \tag{10.9}$$

$$S_z |s, m_s\rangle = \hbar m_s |s, m_s\rangle . \tag{10.10}$$

The spin quantum number s is dimensionless. For spin one-half,

$$s = \frac{1}{2}, \tag{10.11}$$

while the magnitude of the spin angular momentum is

$$|\boldsymbol{S}| = \sqrt{s(s+1)}\hbar = \frac{\sqrt{3}}{2}\hbar. \tag{10.12}$$

It is therefore imprecise to say “the spin equals $\hbar/2$”; $\hbar/2$ is the magnitude of a measured component along any chosen axis, not the magnitude of the vector operator.

10.5 Pauli matrices

For $s = 1/2$,

$$S_i = \frac{\hbar}{2}\sigma_i, \tag{10.13}$$

where

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{10.14}$$

They satisfy

$$\boxed{\sigma_i \sigma_j = \delta_{ij} I + \mathrm{i}\epsilon_{ijk}\sigma_k}, \tag{10.15}$$

so

$$[\sigma_i, \sigma_j] = 2\mathrm{i}\epsilon_{ijk}\sigma_k, \tag{10.16}$$

$$\{\sigma_i, \sigma_j\} = 2\delta_{ij} I. \tag{10.17}$$

For arbitrary vectors $\boldsymbol{a}, \boldsymbol{b}$,

$$(\boldsymbol{a} \cdot \boldsymbol{\sigma})(\boldsymbol{b} \cdot \boldsymbol{\sigma}) = (\boldsymbol{a} \cdot \boldsymbol{b}) I + \mathrm{i}(\boldsymbol{a} \times \boldsymbol{b}) \cdot \boldsymbol{\sigma}. \tag{10.18}$$

10.6 Spin along an arbitrary direction

Let

$$\hat{\boldsymbol{n}} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta). \tag{10.19}$$

The operator

$$S_{\hat{\boldsymbol{n}}} = \frac{\hbar}{2}\hat{\boldsymbol{n}}\cdot\boldsymbol{\sigma} \tag{10.20}$$

has eigenvalues $\pm\hbar/2$. A standard normalized eigenbasis is

$$\boxed{|\hat{\boldsymbol{n}},+\rangle = \begin{pmatrix} \cos(\theta/2) \\ \mathrm{e}^{\mathrm{i}\phi}\sin(\theta/2) \end{pmatrix}}, \tag{10.21}$$

$$\boxed{|\hat{\boldsymbol{n}},-\rangle = \begin{pmatrix} -\mathrm{e}^{-\mathrm{i}\phi}\sin(\theta/2) \\ \cos(\theta/2) \end{pmatrix}}. \tag{10.22}$$

Equivalent expressions differing by overall phases are physically identical.

10.7 Expectation value of spin

For the pure state $|\hat{\boldsymbol{n}},+\rangle$,

$$\langle\boldsymbol{\sigma}\rangle = \hat{\boldsymbol{n}}, \tag{10.23}$$

so

$$\boxed{\langle\boldsymbol{S}\rangle = \frac{\hbar}{2}\hat{\boldsymbol{n}}}. \tag{10.24}$$

Although the expectation value has magnitude $\hbar/2$, the eigenvalue of S^2 is $3\hbar^2/4$.

10.8 General spin-$1/2$ density matrix and the Bloch sphere

Every 2×2 density matrix can be written uniquely as

$$\boxed{\rho = \frac{1}{2}(I + \boldsymbol{r}\cdot\boldsymbol{\sigma})}, \tag{10.25}$$

where $\boldsymbol{r}\in\mathbb{R}^3$ is the Bloch vector. Positivity requires

$$|\boldsymbol{r}| \le 1. \tag{10.26}$$

Its eigenvalues are

$$\lambda_\pm = \frac{1\pm|\boldsymbol{r}|}{2}. \tag{10.27}$$

Therefore

$$|\boldsymbol{r}| = 1 \quad\Longleftrightarrow\quad \rho \text{ is pure}, \tag{10.28}$$

while

$$|\boldsymbol{r}| < 1 \quad\Longleftrightarrow\quad \rho \text{ is mixed}. \tag{10.29}$$

The purity is

$$\operatorname{Tr}\rho^2 = \frac{1+|\boldsymbol{r}|^2}{2}. \tag{10.30}$$

The spin expectation value is

$$\langle\boldsymbol{S}\rangle = \frac{\hbar}{2}\boldsymbol{r}. \tag{10.31}$$

10.9 Populations and coherences for a qubit

In the S_z basis,

$$\rho = \begin{pmatrix} \rho_{++} & \rho_{+-} \\ \rho_{-+} & \rho_{--} \end{pmatrix}. \tag{10.32}$$

The populations are ρ_{++}, ρ_{--} and the coherences are ρ_{+-}, ρ_{-+}. In terms of the Bloch vector,

$$\rho = \frac{1}{2}\begin{pmatrix} 1 + r_z & r_x - \mathrm{i}r_y \\ r_x + \mathrm{i}r_y & 1 - r_z \end{pmatrix}. \tag{10.33}$$

Thus

$$r_z = \rho_{++} - \rho_{--}, \tag{10.34}$$

and transverse spin polarization is encoded in the off-diagonal coherences.

10.10 Unpolarized spin-1/2 ensemble

An isotropic ensemble has

$$\rho_{\text{unpol}} = \frac{1}{2}I, \tag{10.35}$$

so

$$\langle S_x \rangle = \langle S_y \rangle = \langle S_z \rangle = 0. \tag{10.36}$$

No normalized spinor can produce $\rho = I/2$ as a pure-state projector, because

$$\mathrm{Tr}[(I/2)^2] = \frac{1}{2} < 1. \tag{10.37}$$

10.11 Spin in a magnetic field

For a magnetic moment proportional to spin,

$$\boldsymbol{\mu} = \gamma \boldsymbol{S}, \tag{10.38}$$

the Zeeman Hamiltonian is

$$H = -\boldsymbol{\mu} \cdot \boldsymbol{B} = -\gamma \boldsymbol{S} \cdot \boldsymbol{B}. \tag{10.39}$$

The sign of γ depends on the particle. For an electron,

$$\boldsymbol{\mu}_s = -g\mu_B \frac{\boldsymbol{S}}{\hbar} \tag{10.40}$$

with $g \approx 2$, so its gyromagnetic ratio is negative. It is therefore safest to keep γ explicit rather than silently assigning a positive sign.

For a field along z,

$$H = -\frac{\gamma \hbar B}{2}\sigma_z. \tag{10.41}$$

At thermal equilibrium,

$$\rho_\beta = \frac{\mathrm{e}^{-\beta H}}{Z}, \tag{10.42}$$

which gives a longitudinal polarization

$$\langle S_z \rangle = \frac{\hbar}{2}\tanh\left(\frac{\beta\gamma\hbar B}{2}\right) \tag{10.43}$$

when the Hamiltonian is written as $H = -(\gamma\hbar B/2)\sigma_z$. The sign follows the chosen γ.

10.12 Sequential spin measurements

If a spin prepared in $|\hat{\boldsymbol{n}}, +\rangle$ is measured along $\hat{\boldsymbol{m}}$, the probability of obtaining $+\hbar/2$ is

$$\boxed{P(+_{\hat{m}}|+_{\hat{n}}) = |\langle \hat{\boldsymbol{m}}, +|\hat{\boldsymbol{n}}, +\rangle|^2 = \frac{1 + \hat{\boldsymbol{m}} \cdot \hat{\boldsymbol{n}}}{2}} = \cos^2 \frac{\Theta}{2}, \tag{10.44}$$

where Θ is the angle between the directions. The probability of $-\hbar/2$ is

$$\sin^2 \frac{\Theta}{2}. \tag{10.45}$$

This compactly describes Stern–Gerlach sequences.

10.13 Two spin-1/2 particles

The four-dimensional product space is spanned by

$$|{+}{+}\rangle, |{+}{-}\rangle, |{-}{+}\rangle, |{-}{-}\rangle. \tag{10.46}$$

Equivalently, one may use total spin $\boldsymbol{S} = \boldsymbol{S}_1 + \boldsymbol{S}_2$. The triplet and singlet states are

$$|1, 1\rangle = |{+}{+}\rangle, \tag{10.47}$$

$$|1, 0\rangle = \frac{1}{\sqrt{2}}(|{+}{-}\rangle + |{-}{+}\rangle), \tag{10.48}$$

$$|1, -1\rangle = |{-}{-}\rangle, \tag{10.49}$$

$$|0, 0\rangle = \frac{1}{\sqrt{2}}(|{+}{-}\rangle - |{-}{+}\rangle). \tag{10.50}$$

The operators

$$\{S^2, S_z\} \tag{10.51}$$

form a CSCO on this coupled space; alternatively

$$\{S_{1z}, S_{2z}\} \tag{10.52}$$

label the product basis.

10.14 Spin–spin scalar product

Using

$$S^2 = S_1^2 + S_2^2 + 2\boldsymbol{S}_1 \cdot \boldsymbol{S}_2, \tag{10.53}$$

for two spin-one-half particles,

$$\boldsymbol{S}_1 \cdot \boldsymbol{S}_2 = \begin{cases} \hbar^2/4, & S = 1, \\ -3\hbar^2/4, & S = 0. \end{cases} \tag{10.54}$$

This makes the singlet/triplet basis especially useful for Hamiltonians of Heisenberg form

$$H = J\, \boldsymbol{S}_1 \cdot \boldsymbol{S}_2. \tag{10.55}$$

Chapter 11

Orbital Angular Momentum, Spherical Harmonics, and Rotations

11.1 Orbital angular momentum in Cartesian coordinates

Orbital angular momentum is

$$\boldsymbol{L} = \boldsymbol{r} \times \boldsymbol{p}. \tag{11.1}$$

Thus

$$L_x = yp_z - zp_y, \tag{11.2}$$
$$L_y = zp_x - xp_z, \tag{11.3}$$
$$L_z = xp_y - yp_x. \tag{11.4}$$

In the position representation,

$$\boldsymbol{L} = -\mathrm{i}\hbar \boldsymbol{r} \times \boldsymbol{\nabla}. \tag{11.5}$$

The commutators are

$$[L_i, L_j] = \mathrm{i}\hbar \epsilon_{ijk} L_k. \tag{11.6}$$

11.2 Spherical-coordinate representation

With

$$x = r \sin\theta \cos\phi, \qquad y = r \sin\theta \sin\phi, \qquad z = r\cos\theta, \tag{11.7}$$

one finds

$$\boxed{L_z = -\mathrm{i}\hbar \frac{\partial}{\partial \phi}}. \tag{11.8}$$

The ladder operators are

$$\boxed{L_\pm = \hbar \mathrm{e}^{\pm \mathrm{i}\phi} \left(\pm \frac{\partial}{\partial \theta} + \mathrm{i} \cot\theta \frac{\partial}{\partial \phi} \right)}. \tag{11.9}$$

The Casimir operator is

$$\boxed{L^2 = -\hbar^2 \left[\frac{1}{\sin\theta} \frac{\partial}{\partial \theta} \left(\sin\theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial \phi^2} \right]}. \tag{11.10}$$

11.3 Spherical harmonics

The common eigenfunctions of L^2 and L_z are spherical harmonics:

$$L^2 Y_\ell^m = \hbar^2 \ell(\ell+1) Y_\ell^m, \tag{11.11}$$

$$L_z Y_\ell^m = \hbar m Y_\ell^m, \tag{11.12}$$

where

$$\ell = 0, 1, 2, \ldots, \qquad m = -\ell, -\ell+1, \ldots, \ell. \tag{11.13}$$

They are orthonormal on the unit sphere:

$$\int_0^{2\pi} \mathrm{d}\phi \int_0^{\pi} \sin\theta \, \mathrm{d}\theta \, Y_\ell^{m*}(\theta,\phi) Y_{\ell'}^{m'}(\theta,\phi) = \delta_{\ell\ell'}\delta_{mm'}. \tag{11.14}$$

Completeness may be written as

$$\sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} Y_\ell^m(\Omega) Y_\ell^{m*}(\Omega') = \delta(\Omega - \Omega'), \tag{11.15}$$

where

$$\delta(\Omega - \Omega') = \delta(\phi - \phi')\delta(\cos\theta - \cos\theta'). \tag{11.16}$$

11.4 Associated Legendre functions

With the Condon–Shortley convention,

$$\boxed{Y_\ell^m(\theta,\phi) = \sqrt{\frac{2\ell+1}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}} P_\ell^m(\cos\theta) \mathrm{e}^{\mathrm{i}m\phi}} \tag{11.17}$$

for $m \geq 0$, with

$$P_\ell^m(x) = (-1)^m (1-x^2)^{m/2} \frac{\mathrm{d}^m P_\ell(x)}{\mathrm{d}x^m}. \tag{11.18}$$

Negative-m harmonics satisfy

$$\boxed{Y_\ell^{-m} = (-1)^m Y_\ell^{m*}}. \tag{11.19}$$

11.5 Ladder action on spherical harmonics

The general ladder formula becomes

$$\boxed{L_\pm Y_\ell^m = \hbar \sqrt{(\ell \mp m)(\ell \pm m + 1)} Y_\ell^{m\pm 1}}. \tag{11.20}$$

Starting from

$$Y_\ell^\ell(\theta,\phi) \propto \sin^\ell\theta \, \mathrm{e}^{\mathrm{i}\ell\phi}, \tag{11.21}$$

one obtains the full multiplet by lowering.

11.6 Low-order spherical harmonics

Useful examples are

$$Y_0^0 = \frac{1}{\sqrt{4\pi}}, \tag{11.22}$$

$$Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos\theta, \tag{11.23}$$

$$Y_1^{\pm 1} = \mp\sqrt{\frac{3}{8\pi}}\sin\theta\,\mathrm{e}^{\pm \mathrm{i}\phi}, \tag{11.24}$$

$$Y_2^0 = \sqrt{\frac{5}{16\pi}}(3\cos^2\theta - 1), \tag{11.25}$$

$$Y_2^{\pm 1} = \mp\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta\,\mathrm{e}^{\pm \mathrm{i}\phi}, \tag{11.26}$$

$$Y_2^{\pm 2} = \sqrt{\frac{15}{32\pi}}\sin^2\theta\,\mathrm{e}^{\pm 2\mathrm{i}\phi}. \tag{11.27}$$

11.7 Parity of spherical harmonics

Under inversion,

$$\boldsymbol{r} \to -\boldsymbol{r} \tag{11.28}$$

corresponds to

$$(\theta, \phi) \to (\pi - \theta, \phi + \pi). \tag{11.29}$$

Spherical harmonics obey

$$\boxed{Y_\ell^m(\pi - \theta, \phi + \pi) = (-1)^\ell Y_\ell^m(\theta, \phi)}. \tag{11.30}$$

Therefore an orbital state with angular momentum ℓ has parity $(-1)^\ell$.

11.8 Rotations and their generators

A finite active rotation by angle α about unit vector $\hat{\boldsymbol{n}}$ is represented by

$$\boxed{U(R) = \exp\left(-\frac{\mathrm{i}\alpha}{\hbar}\hat{\boldsymbol{n}} \cdot \boldsymbol{J}\right)}. \tag{11.31}$$

For orbital rotations,

$$\boldsymbol{J} = \boldsymbol{L}. \tag{11.32}$$

For spin or total rotations, the relevant angular momentum is the full generator.
Infinitesimally,

$$U(R) = I - \frac{\mathrm{i}}{\hbar}\delta\boldsymbol{\theta} \cdot \boldsymbol{J} + O(\delta\theta^2). \tag{11.33}$$

If $\boldsymbol{V}$ is a vector operator, then with this active-state convention,

$$\boxed{U^\dagger(R)\boldsymbol{V}U(R) = R\boldsymbol{V}}. \tag{11.34}$$

Equivalently, $U(R)\boldsymbol{V}U^\dagger(R) = R^{-1}\boldsymbol{V}$. This is equivalent infinitesimally to

$$[J_i, V_j] = \mathrm{i}\hbar\epsilon_{ijk}V_k. \tag{11.35}$$

11.9 Rotation about the z axis

Since $J_z \left|j, m\right\rangle = \hbar m \left|j, m\right\rangle$,

$$U_z(\alpha) \left|j, m\right\rangle = \mathrm{e}^{-\mathrm{i}m\alpha} \left|j, m\right\rangle . \tag{11.36}$$

For orbital wave functions,

$$\left[U_z(\alpha)\psi\right](r, \theta, \phi) = \psi(r, \theta, \phi - \alpha), \tag{11.37}$$

consistent with the active-rotation convention.

11.10 Spin-$1/2$ rotation formula

For $J_i = (\hbar/2)\sigma_i$,

$$U(\hat{\boldsymbol{n}}, \alpha) = \exp\left(-\frac{\mathrm{i}\alpha}{2}\hat{\boldsymbol{n}} \cdot \boldsymbol{\sigma}\right). \tag{11.38}$$

Since

$$(\hat{\boldsymbol{n}} \cdot \boldsymbol{\sigma})^2 = I, \tag{11.39}$$

the exponential can be evaluated exactly:

$$\boxed{U(\hat{\boldsymbol{n}}, \alpha) = I \cos\frac{\alpha}{2} - \mathrm{i}\hat{\boldsymbol{n}} \cdot \boldsymbol{\sigma} \sin\frac{\alpha}{2}}. \tag{11.40}$$

A 2π rotation gives $U = -I$ for spin one-half, while a 4π rotation returns the spinor to itself. This sign under 2π rotation has no effect on an isolated state's ray but matters in interference and in composite-state transformations.

11.11 Euler-angle form

A general rotation can be parameterized by Euler angles, for example in the z-y-z convention,

$$U(\alpha, \beta, \gamma) = \mathrm{e}^{-\mathrm{i}\alpha J_z/\hbar}\mathrm{e}^{-\mathrm{i}\beta J_y/\hbar}\mathrm{e}^{-\mathrm{i}\gamma J_z/\hbar}. \tag{11.41}$$

Its matrix elements in a fixed-j basis are the Wigner D-matrices,

$$D^j_{m'm}(\alpha, \beta, \gamma) = \left\langle j, m'\middle|U(\alpha, \beta, \gamma)\middle|j, m\right\rangle . \tag{11.42}$$

Spherical harmonics furnish the $j = \ell$ orbital representation of these rotations.

Chapter 12

Central Potentials, Two-Body Reduction, and the Hydrogen Atom

12.1 Central potentials

Consider

$$H = \frac{\boldsymbol{p}^2}{2\mu} + V(r), \qquad r = |\boldsymbol{r}|. \tag{12.1}$$

Because V depends only on r, the Hamiltonian is rotationally invariant:

$$[H, L_i] = 0, \qquad \left[H, L^2\right] = 0. \tag{12.2}$$

Thus energy eigenstates may be chosen as simultaneous eigenstates of H, L^2, L_z.

12.2 Laplacian in spherical coordinates

The three-dimensional Laplacian is

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}. \tag{12.3}$$

Using the angular-momentum operator,

$$\boxed{\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{L^2}{\hbar^2 r^2}}. \tag{12.4}$$

Hence

$$H = -\frac{\hbar^2}{2\mu}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{L^2}{2\mu r^2} + V(r). \tag{12.5}$$

12.3 A note on radial momentum

A frequent shorthand writes the radial kinetic term as $p_r^2/(2\mu)$. With radial measure $r^2\,\mathrm{d}r$, the differential expression

$$\boxed{p_r = -\mathrm{i}\hbar\left(\frac{\partial}{\partial r} + \frac{1}{r}\right)} \tag{12.6}$$

is formally symmetric on suitable functions and reproduces the radial kinetic term. Its status as a self-adjoint observable on the half-line is subtle; in particular, one should not infer that a globally self-adjoint radial momentum operator exists with all the properties of Cartesian momentum. Algebraically,

$$p_r^2 = -\hbar^2 \left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} \right), \tag{12.7}$$

so

$$H = \frac{p_r^2}{2\mu} + \frac{L^2}{2\mu r^2} + V(r). \tag{12.8}$$

Simply taking $p_r = -\mathrm{i}\hbar\partial_r$ in the $r^2\,\mathrm{d}r$ measure is not Hermitian. After introducing $u(r) = rR(r)$, however, the radial equation uses the ordinary one-dimensional derivative $-\mathrm{i}\hbar\partial_r$ acting on u with measure $\mathrm{d}r$.

12.4 Separation of variables

Write

$$\psi_{E\ell m}(r,\theta,\phi) = R_{E\ell}(r) Y_\ell^m(\theta,\phi). \tag{12.9}$$

Then the radial equation is

$$-\frac{\hbar^2}{2\mu}\left[\frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}R}{\mathrm{d}r}\right) - \frac{\ell(\ell+1)}{r^2}R\right] + V(r)R = ER. \tag{12.10}$$

Defining

$$u(r) = rR(r), \tag{12.11}$$

gives the one-dimensional form

$$\boxed{-\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2u}{\mathrm{d}r^2} + V_{\text{eff}}(r)u = Eu}, \tag{12.12}$$

with effective potential

$$\boxed{V_{\text{eff}}(r) = V(r) + \frac{\hbar^2\ell(\ell+1)}{2\mu r^2}}. \tag{12.13}$$

The second term is the centrifugal barrier.

Normalization is

$$\int_0^\infty |R(r)|^2 r^2\,\mathrm{d}r = 1 \tag{12.14}$$

for a normalized angular function, equivalently

$$\int_0^\infty |u(r)|^2\,\mathrm{d}r = 1. \tag{12.15}$$

Regularity normally requires

$$u(0) = 0. \tag{12.16}$$

12.5 Two-body problem and center-of-mass variables

Consider two particles of masses m_1, m_2 with

$$H = \frac{\boldsymbol{p}_1^2}{2m_1} + \frac{\boldsymbol{p}_2^2}{2m_2} + V(|\boldsymbol{r}_1 - \boldsymbol{r}_2|). \tag{12.17}$$

Define the center-of-mass and relative coordinates

$$\boldsymbol{R} = \frac{m_1\boldsymbol{r}_1 + m_2\boldsymbol{r}_2}{M}, \qquad \boldsymbol{r} = \boldsymbol{r}_1 - \boldsymbol{r}_2, \tag{12.18}$$

where

$$M = m_1 + m_2. \tag{12.19}$$

The conjugate momenta are

$$\boldsymbol{P} = \boldsymbol{p}_1 + \boldsymbol{p}_2, \tag{12.20}$$

$$\boldsymbol{p} = \mu\left(\frac{\boldsymbol{p}_1}{m_1} - \frac{\boldsymbol{p}_2}{m_2}\right) = \frac{m_2\boldsymbol{p}_1 - m_1\boldsymbol{p}_2}{M}, \tag{12.21}$$

with reduced mass

$$\boxed{\mu = \frac{m_1 m_2}{m_1 + m_2}}. \tag{12.22}$$

Then

$$\boxed{H = \frac{\boldsymbol{P}^2}{2M} + \frac{\boldsymbol{p}^2}{2\mu} + V(r)}. \tag{12.23}$$

The center-of-mass and internal motions separate. The internal angular momentum is

$$\boldsymbol{L} = \boldsymbol{r} \times \boldsymbol{p}. \tag{12.24}$$

12.6 The Coulomb problem

For hydrogenic systems,

$$V(r) = -\frac{Ze^2}{4\pi\epsilon_0 r} \equiv -\frac{\kappa}{r}, \tag{12.25}$$

where

$$\kappa = \frac{Ze^2}{4\pi\epsilon_0}. \tag{12.26}$$

The internal Hamiltonian is

$$H = -\frac{\hbar^2}{2\mu}\nabla^2 - \frac{\kappa}{r}. \tag{12.27}$$

For ordinary hydrogen, $Z = 1$ and the reduced mass is very close to, but not exactly equal to, the electron mass.

12.7 Bohr radius and energy scale

Define the reduced-mass Bohr radius

$$\boxed{a_0 = \frac{4\pi\epsilon_0\hbar^2}{\mu e^2}} \tag{12.28}$$

for $Z = 1$. More generally the characteristic radius scales as a_0/Z. The bound-state energy scale is

$$E_{\mathrm{Ry}} = \frac{\mu e^4}{2(4\pi\epsilon_0)^2\hbar^2}. \tag{12.29}$$

12.8 Hydrogenic energy spectrum

Solving the radial equation with normalizability gives

$$\boxed{E_n = -\frac{\mu Z^2 e^4}{2(4\pi\epsilon_0)^2\hbar^2}\frac{1}{n^2}}, \qquad n = 1, 2, 3, \ldots. \tag{12.30}$$

For each principal quantum number n,

$$\ell = 0, 1, \ldots, n-1, \tag{12.31}$$

and

$$m = -\ell, -\ell+1, \ldots, \ell. \tag{12.32}$$

Ignoring spin and relativistic corrections, the Coulomb energy depends only on n, producing an accidental degeneracy larger than that required by ordinary rotational symmetry.

The orbital degeneracy at fixed n is

$$\sum_{\ell=0}^{n-1}(2\ell+1) = n^2. \tag{12.33}$$

Including electron spin doubles this to $2n^2$ before fine-structure effects are considered.

12.9 Dimensionless radial equation

For a bound state $E < 0$, define

$$\kappa_E = \frac{\sqrt{-2\mu E}}{\hbar}, \qquad \rho = 2\kappa_E r. \tag{12.34}$$

The radial solution has asymptotic behavior

$$u(r) \sim r^{\ell+1} \quad (r \to 0), \tag{12.35}$$

$$u(r) \sim \mathrm{e}^{-\kappa_E r} \quad (r \to \infty). \tag{12.36}$$

Thus set

$$u(\rho) = \rho^{\ell+1}\mathrm{e}^{-\rho/2}v(\rho). \tag{12.37}$$

The function v satisfies an associated-Laguerre differential equation. Normalizability requires the series for v to terminate, which quantizes the energy and produces associated Laguerre polynomials.

12.10 Hydrogenic radial functions

A standard normalized form is

$$\boxed{R_{n\ell}(r) = \left(\frac{2Z}{na_0}\right)^{3/2}\sqrt{\frac{(n-\ell-1)!}{2n(n+\ell)!}}\mathrm{e}^{-\rho/2}\rho^\ell L_{n-\ell-1}^{2\ell+1}(\rho)}, \tag{12.38}$$

where

$$\rho = \frac{2Zr}{na_0}. \tag{12.39}$$

The full stationary states are

$$\psi_{n\ell m}(r,\theta,\phi) = R_{n\ell}(r)Y_\ell^m(\theta,\phi). \tag{12.40}$$

12.11 Examples

For $Z = 1$,

$$R_{10}(r) = 2a_0^{-3/2}\mathrm{e}^{-r/a_0}, \tag{12.41}$$

so

$$\psi_{100}(r) = \frac{1}{\sqrt{\pi a_0^3}}\mathrm{e}^{-r/a_0}. \tag{12.42}$$

For the $2s$ state,

$$R_{20}(r) = \frac{1}{2\sqrt{2}\,a_0^{3/2}}\left(2 - \frac{r}{a_0}\right)\mathrm{e}^{-r/(2a_0)}. \tag{12.43}$$

For the $2p$ states,

$$R_{21}(r) = \frac{1}{2\sqrt{6}\,a_0^{3/2}}\frac{r}{a_0}\mathrm{e}^{-r/(2a_0)}. \tag{12.44}$$

The angular dependence is supplied by Y_1^m.

12.12 Degeneracy and hidden symmetry

Rotational invariance alone guarantees degeneracy in m at fixed n, ℓ, because

$$\left[H, L^2\right] = [H, L_z] = 0. \tag{12.45}$$

The additional degeneracy among different ℓ values at fixed n is special to the $1/r$ potential and is associated with the conserved Runge–Lenz vector. This is often called accidental degeneracy because it is not explained by the manifest $SO(3)$ rotational symmetry alone.

Part III

Problems, Solutions , and Assignments

Appendix A

Problems and Solutions

A.1 Bra vectors, inner products, and inequalities

Exercise A.1 (Problem 1: bras and an inner product)**.** Let

$$|\phi\rangle = \begin{pmatrix} 2 \\ -\mathrm{i} \\ 2-3\mathrm{i} \end{pmatrix}, \qquad |\psi\rangle = \begin{pmatrix} -3\mathrm{i} \\ 2+\mathrm{i} \\ 4 \end{pmatrix}. \tag{A.1}$$

Find the corresponding bras and compute $\langle\phi|\psi\rangle$.

Solution.

$$\langle\phi| = \begin{pmatrix} 2 & \mathrm{i} & 2+3\mathrm{i} \end{pmatrix}, \qquad \langle\psi| = \begin{pmatrix} 3\mathrm{i} & 2-\mathrm{i} & 4 \end{pmatrix}. \tag{A.2}$$

Therefore

$$\langle\phi|\psi\rangle = 2(-3\mathrm{i}) + \mathrm{i}(2+\mathrm{i}) + (2+3\mathrm{i})4 \tag{A.3}$$

$$= \boxed{7+8\mathrm{i}}. \tag{A.4}$$

Exercise A.2 (Problem 2: Schwarz and triangle inequalities)**.** Let $|\phi_1\rangle, |\phi_2\rangle$ be orthonormal and

$$|\psi\rangle = 3\mathrm{i}\,|\phi_1\rangle - 7\mathrm{i}\,|\phi_2\rangle, \qquad |\chi\rangle = -|\phi_1\rangle + 2\mathrm{i}\,|\phi_2\rangle. \tag{A.5}$$

Find $|\psi+\chi\rangle$ and its bra, compute $\langle\psi|\chi\rangle$ and $\langle\chi|\psi\rangle$, and verify the Cauchy–Schwarz and triangle inequalities.

Solution.

$$|\psi+\chi\rangle = (-1+3\mathrm{i})\,|\phi_1\rangle - 5\mathrm{i}\,|\phi_2\rangle, \tag{A.6}$$

$$\langle\psi+\chi| = (-1-3\mathrm{i})\,\langle\phi_1| + 5\mathrm{i}\,\langle\phi_2|. \tag{A.7}$$

The scalar products are

$$\langle\psi|\chi\rangle = -14+3\mathrm{i}, \qquad \langle\chi|\psi\rangle = -14-3\mathrm{i} = \langle\psi|\chi\rangle^*. \tag{A.8}$$

Moreover

$$\langle\psi|\psi\rangle = 58, \qquad \langle\chi|\chi\rangle = 5, \qquad |\langle\psi|\chi\rangle|^2 = 205 < 290, \tag{A.9}$$

so Cauchy–Schwarz holds. Also

$$\|\psi+\chi\| = \sqrt{35} \le \sqrt{58} + \sqrt{5} = \|\psi\| + \|\chi\|. \tag{A.10}$$

Exercise A.3 (Problem 3: orthogonality fixes a complex coefficient)**.** Let

$$|\psi_1\rangle = 2\mathrm{i}\,|\phi_1\rangle + |\phi_2\rangle - a\,|\phi_3\rangle + 4\,|\phi_4\rangle\,, \tag{A.11}$$

$$|\psi_2\rangle = 3\,|\phi_1\rangle - \mathrm{i}\,|\phi_2\rangle + 5\,|\phi_3\rangle - |\phi_4\rangle\,, \tag{A.12}$$

where $\{|\phi_i\rangle\}_{i=1}^{4}$ is orthonormal. Find a such that the two states are orthogonal.

Solution. Orthogonality requires

$$\begin{aligned} 0 = \langle\psi_1|\psi_2\rangle &= (-2\mathrm{i})3 + (1)(-\mathrm{i}) + (-a^*)5 + 4(-1) && \text{(A.13)}\\ &= -4 - 7\mathrm{i} - 5a^*. && \text{(A.14)} \end{aligned}$$

Hence

$$a^* = \frac{-4-7\mathrm{i}}{5}, \qquad \boxed{a = \frac{-4+7\mathrm{i}}{5}}. \tag{A.15}$$

A.2 Adjoints, outer products, and projectors

Exercise A.4 (Problem 4: Hermitian combinations and an operator function)**.** For an arbitrary operator A, discuss the Hermiticity of

$$A + A^\dagger, \qquad \mathrm{i}(A + A^\dagger), \qquad \mathrm{i}(A - A^\dagger). \tag{A.16}$$

Also find the adjoint of

$$f(A) = (I + \mathrm{i}A + 3A^2)(I - 2\mathrm{i}A - 9A^2)(5I + 7A)^{-1}, \tag{A.17}$$

assuming the inverse exists.

Solution.

$$(A + A^\dagger)^\dagger = A + A^\dagger, \tag{A.18}$$

so it is Hermitian. On the other hand

$$[\mathrm{i}(A + A^\dagger)]^\dagger = -\mathrm{i}(A + A^\dagger), \tag{A.19}$$

so it is anti-Hermitian, whereas

$$[\mathrm{i}(A - A^\dagger)]^\dagger = \mathrm{i}(A - A^\dagger), \tag{A.20}$$

so it is Hermitian. Writing the three factors in their displayed order,

$$\boxed{f(A)^\dagger = (5I + 7A^\dagger)^{-1}(I + 2\mathrm{i}A^\dagger - 9(A^\dagger)^2)(I - \mathrm{i}A^\dagger + 3(A^\dagger)^2)}. \tag{A.21}$$

If $A = A^\dagger$, all factors are functions of the same operator and therefore commute, allowing their order to be rearranged.

Exercise A.5 (Problem 5: outer products and traces)**.** Let

$$|\psi\rangle = 9\mathrm{i}\,|\phi_1\rangle + 2\,|\phi_2\rangle\,, \qquad |\chi\rangle = -\frac{\mathrm{i}}{\sqrt{2}}\,|\phi_1\rangle + \frac{1}{\sqrt{2}}\,|\phi_2\rangle\,, \tag{A.22}$$

with $\langle\phi_1|\phi_2\rangle = 0$ and normalized basis states. Compare $|\psi\rangle\langle\chi|$ and $|\chi\rangle\langle\psi|$, find their adjoints and traces, and compare $\mathrm{Tr}\,|\psi\rangle\langle\psi|$ with $\mathrm{Tr}\,|\chi\rangle\langle\chi|$.

Solution. One obtains

$$|\psi\rangle\langle\chi| = -\frac{9}{\sqrt{2}}|\phi_1\rangle\langle\phi_1| + \frac{9\mathrm{i}}{\sqrt{2}}|\phi_1\rangle\langle\phi_2| + \frac{2\mathrm{i}}{\sqrt{2}}|\phi_2\rangle\langle\phi_1| + \frac{2}{\sqrt{2}}|\phi_2\rangle\langle\phi_2|. \tag{A.23}$$

The third term is *positive*; the handwritten solution has a minus sign at this point. As always,

$$(|\psi\rangle\langle\chi|)^\dagger = |\chi\rangle\langle\psi|, \tag{A.24}$$

so the two operators are not equal here. Their traces are

$$\mathrm{Tr}\,|\psi\rangle\langle\chi| = \langle\chi|\psi\rangle = -\frac{7}{\sqrt{2}}, \tag{A.25}$$

$$\mathrm{Tr}\,|\chi\rangle\langle\psi| = \langle\psi|\chi\rangle = -\frac{7}{\sqrt{2}}, \tag{A.26}$$

which happen to be equal because this overlap is real. Finally,

$$\mathrm{Tr}\,|\psi\rangle\langle\psi| = \langle\psi|\psi\rangle = 85, \qquad \mathrm{Tr}\,|\chi\rangle\langle\chi| = \langle\chi|\chi\rangle = 1. \tag{A.27}$$

Thus $|\chi\rangle\langle\chi|$ is a rank-one projector, whereas $|\psi\rangle\langle\psi|$ is not; the projector onto the ray of ψ is $|\psi\rangle\langle\psi|/85$.

Exercise A.6 (Problem 6: a differential Hermitian operator)**.** Consider on the real line the differential expression

$$A = \mathrm{i}(x^2+1)\frac{\mathrm{d}}{\mathrm{d}x} + \mathrm{i}x. \tag{A.28}$$

Show that it is symmetric on a suitable domain, solve $A\psi = 0$, normalize the solution, and find the probability for $-1 \le x \le 1$.

Solution. Integration by parts shows that the derivative term contributes the extra $2x$ needed to combine with the adjoint of the multiplication term. With boundary conditions such that

$$[(1+x^2)\phi^*(x)\psi(x)]_{-\infty}^{\infty} = 0, \tag{A.29}$$

one has $\langle\phi|A\psi\rangle = \langle A\phi|\psi\rangle$. The eigenvalue equation $A\psi = 0$ gives

$$(1+x^2)\psi'(x) + x\psi(x) = 0, \tag{A.30}$$

so

$$\psi(x) = \frac{C}{\sqrt{1+x^2}}. \tag{A.31}$$

Since

$$\int_{-\infty}^{\infty} \frac{\mathrm{d}x}{1+x^2} = \pi, \tag{A.32}$$

we may take $C = 1/\sqrt{\pi}$. Hence

$$P(-1 \le x \le 1) = \frac{1}{\pi}\int_{-1}^{1} \frac{\mathrm{d}x}{1+x^2} = \boxed{\frac{1}{2}}. \tag{A.33}$$

The word "Hermitian" here presupposes an appropriate operator domain; the differential expression alone is not enough to establish self-adjointness.

Exercise A.7 (Problem 7: a two-level Hamiltonian)**.** Let

$$H = a\left(|\phi_1\rangle\langle\phi_2| + |\phi_2\rangle\langle\phi_1|\right), \qquad a \in \mathbb{R}, \tag{A.34}$$

where $|\phi_1\rangle, |\phi_2\rangle$ form a complete orthonormal basis. Determine H^2, decide whether the basis vectors are energy eigenstates, find the normalized energy eigenstates and eigenvalues, and write the matrix of H.

Solution.

$$H^2 = a^2 \left(|\phi_1\rangle\langle\phi_1| + |\phi_2\rangle\langle\phi_2| \right) = a^2 I. \tag{A.35}$$

Therefore $H^2/a^2 = I$, which is itself a projector. The original basis vectors are exchanged,

$$H\,|\phi_1\rangle = a\,|\phi_2\rangle\,, \qquad H\,|\phi_2\rangle = a\,|\phi_1\rangle\,, \tag{A.36}$$

so neither is an eigenvector. Instead

$$|E_+\rangle = \frac{|\phi_1\rangle + |\phi_2\rangle}{\sqrt{2}}, \qquad E_+ = a, \tag{A.37}$$

$$|E_-\rangle = \frac{|\phi_1\rangle - |\phi_2\rangle}{\sqrt{2}}, \qquad E_- = -a. \tag{A.38}$$

In the $\{\phi_1, \phi_2\}$ basis,

$$H = a \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{A.39}$$

A.3 Energy measurements and two-state oscillations

Exercise A.8 (Problem 8: an unnormalized superposition)**.** Let $H\,|\phi_n\rangle = nE_0\,|\phi_n\rangle$ for $n = 1, \ldots, 5$, and consider

$$|\psi\rangle = \frac{1}{\sqrt{19}}\,|\phi_1\rangle + \frac{2}{\sqrt{19}}\,|\phi_2\rangle + \sqrt{\frac{2}{19}}\,|\phi_3\rangle + \sqrt{\frac{3}{19}}\,|\phi_4\rangle + \sqrt{\frac{5}{19}}\,|\phi_5\rangle\,. \tag{A.40}$$

Find the energy probabilities and the mean energy.

Solution. The state as written is not normalized:

$$\langle\psi|\psi\rangle = \frac{15}{19}. \tag{A.41}$$

Thus the physical probabilities are obtained after dividing the squared amplitudes by 15/19:

$$(p_1, p_2, p_3, p_4, p_5) = \frac{1}{15}(1, 4, 2, 3, 5). \tag{A.42}$$

Consequently

$$\boxed{\langle H\rangle = E_0 \frac{1 + 2(4) + 3(2) + 4(3) + 5(5)}{15} = \frac{52}{15} E_0}. \tag{A.43}$$

Exercise A.9 (Problem 9: oscillation between two bases)**.** Let $|m_1\rangle, |m_2\rangle$ be Hamiltonian eigenstates with energies E_1, E_2, and define

$$|\psi_1\rangle = \cos\theta\,|m_1\rangle - \sin\theta\,|m_2\rangle\,, \tag{A.44}$$

$$|\psi_2\rangle = \sin\theta\,|m_1\rangle + \cos\theta\,|m_2\rangle\,. \tag{A.45}$$

If the system begins in $|\psi_1\rangle$, find the survival and transition probabilities.

Solution. Time evolution gives

$$|\psi(t)\rangle = \cos\theta\,\mathrm{e}^{-\mathrm{i}E_1 t/\hbar}\,|m_1\rangle - \sin\theta\,\mathrm{e}^{-\mathrm{i}E_2 t/\hbar}\,|m_2\rangle\,. \tag{A.46}$$

With $\Delta E = E_2 - E_1$,

$$\boxed{P_{1\to2}(t) = \sin^2(2\theta)\sin^2\left(\frac{\Delta E\, t}{2\hbar}\right)}, \tag{A.47}$$

$$\boxed{P_{1\to1}(t) = 1 - P_{1\to2}(t)}. \tag{A.48}$$

The factors of $\hbar$ in the dynamical phases are essential.

A.4 Matrices, projectors, and Ehrenfest dynamics

Exercise A.10 (Problem 10: a matrix Hamiltonian and an energy projector)**.** Consider

$$H = \begin{pmatrix} 2 & \mathrm{i} & 0 \\ -\mathrm{i} & 1 & 1 \\ 0 & 1 & 0 \end{pmatrix}. \tag{A.49}$$

Is $|\lambda\rangle = (\mathrm{i}, 7\mathrm{i}, -2)^T$ an eigenvector? Is H Hermitian? If $|a_1\rangle$ is a normalized energy eigenvector, show that $P = |a_1\rangle\langle a_1|$ is a projector and evaluate $[P, H]$.

Solution. Direct multiplication gives

$$H\,|\lambda\rangle = \begin{pmatrix} -7 + 2\mathrm{i} \\ -1 + 7\mathrm{i} \\ 7\mathrm{i} \end{pmatrix}, \tag{A.50}$$

which is not proportional to $|\lambda\rangle$, so it is not an eigenvector. The matrix obeys $H^\dagger = H$. For normalized $|a_1\rangle$,

$$P^2 = P, \qquad P^\dagger = P. \tag{A.51}$$

If $H\,|a_1\rangle = E_1\,|a_1\rangle$, Hermiticity also gives $\langle a_1|\,H = E_1\,\langle a_1|$, and therefore

$$\boxed{[P, H] = 0}. \tag{A.52}$$

Exercise A.11 (Problem 11: driven harmonic oscillator)**.** For

$$H = \frac{P^2}{2m} + \frac{1}{2}kX^2 + qE_0X\cos\omega t, \tag{A.53}$$

find $\mathrm{d}\langle X\rangle/\,\mathrm{d}t$, $\mathrm{d}\langle P\rangle/\,\mathrm{d}t$, and $\mathrm{d}\langle H\rangle/\,\mathrm{d}t$, and solve for $\langle X\rangle(t)$.

Solution. With $\omega_0 = \sqrt{k/m}$,

$$\frac{\mathrm{d}\langle X\rangle}{\mathrm{d}t} = \frac{\langle P\rangle}{m}, \qquad \frac{\mathrm{d}\langle P\rangle}{\mathrm{d}t} = -k\langle X\rangle - qE_0\cos\omega t, \tag{A.54}$$

$$\boxed{\frac{\mathrm{d}\langle H\rangle}{\mathrm{d}t} = -qE_0\omega\sin\omega t\,\langle X\rangle}. \tag{A.55}$$

Thus

$$\ddot{x} + \omega_0^2 x = -\frac{qE_0}{m}\cos\omega t, \qquad x(t) = \langle X\rangle(t). \tag{A.56}$$

The handwritten problem specifies only $x(0) = x_0$; a second initial condition is required. If $\dot{x}(0) = v_0$, then for $\omega \neq \omega_0$,

$$\boxed{x(t) = \left[x_0 + \frac{qE_0/m}{\omega_0^2 - \omega^2}\right]\cos\omega_0 t + \frac{v_0}{\omega_0}\sin\omega_0 t - \frac{qE_0/m}{\omega_0^2 - \omega^2}\cos\omega t}. \tag{A.57}$$

Exercise A.12 (Problem 12: energy measurement followed by another observable)**.** Let

$$H = \epsilon_0\begin{pmatrix} 1 & -1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \qquad A = a\begin{pmatrix} 0 & 4 & 0 \\ 4 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}. \tag{A.58}$$

Find the energy eigenvalues. If the energy result is $-\epsilon_0$, find the probabilities for a subsequent measurement of A and the uncertainty ΔA.

Solution. The energy eigenvalues are

$$0, \quad -\epsilon_0, \quad 2\epsilon_0, \tag{A.59}$$

with a convenient normalized eigenbasis

$$|E=0\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\\0\end{pmatrix}, \quad |E=-\epsilon_0\rangle = \begin{pmatrix}0\\0\\1\end{pmatrix}, \quad |E=2\epsilon_0\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}-1\\1\\0\end{pmatrix}. \tag{A.60}$$

The eigenvalues of A are

$$-\sqrt{17}\,a, \qquad 0, \qquad +\sqrt{17}\,a. \tag{A.61}$$

Corresponding normalized eigenvectors can be chosen as

$$\frac{1}{\sqrt{34}}\begin{pmatrix}4\\-\sqrt{17}\\1\end{pmatrix}, \quad \frac{1}{\sqrt{17}}\begin{pmatrix}1\\0\\-4\end{pmatrix}, \quad \frac{1}{\sqrt{34}}\begin{pmatrix}4\\\sqrt{17}\\1\end{pmatrix}. \tag{A.62}$$

After measuring $-\epsilon_0$ the state is $(0,0,1)^T$, so

$$\boxed{P(-\sqrt{17}a) = \frac{1}{34}, \quad P(0) = \frac{16}{17}, \quad P(+\sqrt{17}a) = \frac{1}{34}}. \tag{A.63}$$

In that state $\langle A\rangle = 0$ and $\langle A^2\rangle = a^2$, hence

$$\boxed{\Delta A = |a|}. \tag{A.64}$$

(If the parameter a is assumed positive, this is simply a.)

A.5 Wave functions, current, and operator identities

Exercise A.13 (Problem 13: infer a potential from a stationary wave)**.** Inside $0 \le x \le a$, let

$$\psi(x,t) = \sin\left(\frac{\pi x}{a}\right) \mathrm{e}^{-\mathrm{i}\omega t}. \tag{A.65}$$

Find the potential inside the well and the probability for $a/4 \le x \le 3a/4$.

Solution. Substitution into the Schrödinger equation gives a constant interior potential

$$\boxed{V_0 = \hbar\omega - \frac{\hbar^2\pi^2}{2ma^2}}. \tag{A.66}$$

If confinement is meant literally, the potential is infinite outside $[0,a]$. The supplied wave function is not normalized, so use a ratio of integrals:

$$P = \frac{\displaystyle\int_{a/4}^{3a/4} \sin^2(\pi x/a)\,\mathrm{d}x}{\displaystyle\int_0^a \sin^2(\pi x/a)\,\mathrm{d}x} = \boxed{\frac{2+\pi}{2\pi}}. \tag{A.67}$$

Exercise A.14 (Problem 14: infinite-well superposition and current)**.** A particle in a one-dimensional infinite well $0 < x < a$ is given at $t = 0$ by

$$\psi(x,0) = \sqrt{\frac{3}{5a}}\sin\frac{3\pi x}{a} + \frac{1}{\sqrt{5a}}\sin\frac{5\pi x}{a}. \tag{A.68}$$

Find its time evolution, probability density and probability current, and verify the continuity equation.

Solution. The state as written has norm 2/5, not one. A normalized version is

$$\psi(x,0) = \frac{\sqrt{3}}{2}\phi_3(x) + \frac{1}{2}\phi_5(x), \qquad \phi_n(x) = \sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a}. \tag{A.69}$$

Thus

$$\psi(x,t) = \frac{\sqrt{3}}{2}\phi_3(x)\mathrm{e}^{-\mathrm{i}E_3 t/\hbar} + \frac{1}{2}\phi_5(x)\mathrm{e}^{-\mathrm{i}E_5 t/\hbar}, \tag{A.70}$$

where

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}. \tag{A.71}$$

For real ϕ_n,

$$\rho = \frac{3}{4}\phi_3^2 + \frac{1}{4}\phi_5^2 + \frac{\sqrt{3}}{2}\phi_3\phi_5\cos\left(\frac{E_5 - E_3}{\hbar}t\right), \tag{A.72}$$

while

$$\boxed{J = \frac{\hbar\sqrt{3}}{4m}\left(\phi_5\phi_3' - \phi_3\phi_5'\right)\sin\left(\frac{E_5 - E_3}{\hbar}t\right)}. \tag{A.73}$$

Using the stationary Schrödinger equations for ϕ_3 and ϕ_5, or differentiating directly, gives

$$\frac{\partial\rho}{\partial t} + \frac{\partial J}{\partial x} = 0. \tag{A.74}$$

The same equation also holds for the unnormalized state; both ρ and J are simply scaled by the common norm factor.

Exercise A.15 (Problem 15: when is $(A + \mathrm{i}B)/\sqrt{A^2 + B^2}$ unitary?)**.** Consider

$$U = (A + \mathrm{i}B)(A^2 + B^2)^{-1/2}. \tag{A.75}$$

Give sufficient conditions for U to be unitary.

Solution. If

$$A = A^\dagger, \qquad B = B^\dagger, \qquad [A, B] = 0, \tag{A.76}$$

and $A^2 + B^2$ has no zero eigenvalue on the space under consideration, then its positive square root $D = (A^2 + B^2)^{1/2}$ commutes with A, B, and

$$U^\dagger = D^{-1}(A - \mathrm{i}B). \tag{A.77}$$

Therefore

$$U^\dagger U = D^{-2}(A - \mathrm{i}B)(A + \mathrm{i}B) = D^{-2}(A^2 + B^2) = I, \tag{A.78}$$

and similarly $UU^\dagger = I$. If D has a kernel, the expression instead defines at best a partial isometry on its support unless the zero modes are treated separately.

Exercise A.16 (Problem 16: an exponential commutator)**.** Evaluate $[\mathrm{e}^{\mathrm{i}x}, p]$ given $[x, p] = \mathrm{i}\hbar$.

Solution. For any sufficiently regular $f(x)$,

$$[f(x), p] = \mathrm{i}\hbar f'(x). \tag{A.79}$$

Hence

$$\boxed{[\mathrm{e}^{\mathrm{i}x}, p] = -\hbar\mathrm{e}^{\mathrm{i}x}}. \tag{A.80}$$

The formula $[x, p^n] = \mathrm{i}\hbar n p^{n-1}$ written below this question in the source is true, but it is not the requested commutator.

Exercise A.17 (Problem 17: derivative operators on the sphere)**.** Let

$$\psi(\theta,\phi) = \mathrm{e}^{-3\mathrm{i}\phi}\cos\theta, \qquad A_\phi = \frac{\partial}{\partial\phi}, \qquad B_\theta = \frac{\partial}{\partial\theta}. \tag{A.81}$$

Determine whether ψ is an eigenfunction of either operator, discuss Hermiticity using the spherical inner product, calculate the expectation values, and find the commutator.

Solution. Since

$$A_\phi\psi = -3\mathrm{i}\psi, \tag{A.82}$$

ψ is an eigenfunction of A_ϕ with eigenvalue $-3\mathrm{i}$. This already shows that A_ϕ itself is not Hermitian; with periodic boundary conditions it is anti-Hermitian, while $-\mathrm{i}\partial_\phi$ is Hermitian. By contrast,

$$B_\theta\psi = -\mathrm{e}^{-3\mathrm{i}\phi}\sin\theta \tag{A.83}$$

is not proportional to ψ. With the measure $\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi$,

$$\left(\frac{\partial}{\partial\theta}\right)^\dagger = -\frac{\partial}{\partial\theta} - \cot\theta \tag{A.84}$$

(up to boundary-domain qualifications), so B_θ is not Hermitian either. After normalizing ψ,

$$\langle A_\phi\rangle = -3\mathrm{i}, \qquad \langle B_\theta\rangle = 0. \tag{A.85}$$

Finally the partial derivatives commute on smooth functions:

$$\boxed{[A_\phi, B_\theta] = 0}. \tag{A.86}$$

Appendix B

Assignments

1. Prove

$$[AB, CD] = -AC\{D, B\} + A\{C, B\}D - C\{D, A\}B + \{C, A\}DB. \tag{B.1}$$

2. Suppose a 2×2 matrix X (not necessarily Hermitian or unitary) is written as

$$X = a_0 I + \boldsymbol{\sigma} \cdot \boldsymbol{a}. \tag{B.2}$$

(a) Relate a_0 and a_k $(k = 1, 2, 3)$ to $\operatorname{Tr} X$ and $\operatorname{Tr}(\sigma_k X)$.

(b) Obtain a_0 and a_k explicitly in terms of the entries X_{ij}.

3. Using bra-ket algebra, prove

$$\operatorname{Tr}(XY) = \operatorname{Tr}(YX), \qquad (XY)^\dagger = Y^\dagger X^\dagger. \tag{B.3}$$

4. With $|+\rangle, |-\rangle$ orthonormal and

$$S_x = \frac{\hbar}{2}(|+\rangle\langle-| + |-\rangle\langle+|), \tag{B.4}$$

$$S_y = \frac{\mathrm{i}\hbar}{2}(-|+\rangle\langle-| + |-\rangle\langle+|), \tag{B.5}$$

$$S_z = \frac{\hbar}{2}(|+\rangle\langle+| - |-\rangle\langle-|), \tag{B.6}$$

prove

$$[S_i, S_j] = \mathrm{i}\hbar\epsilon_{ijk}S_k, \qquad \{S_i, S_j\} = \frac{\hbar^2}{2}\delta_{ij}I. \tag{B.7}$$

5. For

$$H = a(|1\rangle\langle1| - |2\rangle\langle2| + |1\rangle\langle2| + |2\rangle\langle1|), \tag{B.8}$$

find the energy eigenvalues and normalized eigenkets.

6. Consider

$$H = H_{11}|1\rangle\langle1| + H_{22}|2\rangle\langle2| + H_{12}(|1\rangle\langle2| + |2\rangle\langle1|), \tag{B.9}$$

with real H_{ij}. Find the energy eigenvalues and eigenkets and verify the $H_{12} = 0$ limit.

7. Find the normalized eigenvectors and eigenvalues of

$$\frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \tag{B.10}$$

discuss degeneracy, and give a physical example.

8. Let two Hermitian operators anticommute, $\{A, B\} = 0$. Discuss whether they can possess a common eigenket and state the exceptional cases carefully.

9. Let $[A_1, A_2] \neq 0$ but $[A_1, H] = [A_2, H] = 0$. Explain why this generally implies degeneracy of the energy eigenspaces, identify the exception, and illustrate with the central-force Hamiltonian $H = p^2/(2m) + V(r)$ and $A_1 = L_z$, $A_2 = L_x$.

10. Verify, for functions representable by suitable power series,

$$[x_i, G(\boldsymbol{p})] = \mathrm{i}\hbar\frac{\partial G}{\partial p_i}, \qquad [p_i, F(\boldsymbol{x})] = -\mathrm{i}\hbar\frac{\partial F}{\partial x_i}, \tag{B.11}$$

and evaluate $[x^2, p^2]$. Compare with the classical Poisson bracket.

11. For the finite translation operator

$$\mathcal{T}(\boldsymbol{\ell}) = \exp\left(-\frac{\mathrm{i}}{\hbar}\boldsymbol{p}\cdot\boldsymbol{\ell}\right), \tag{B.12}$$

find $[x_i, \mathcal{T}(\boldsymbol{\ell})]$ and determine how $\langle \boldsymbol{x} \rangle$ changes under translation.

12. Prove

$$\langle p'|x|\alpha\rangle = \mathrm{i}\hbar\frac{\partial}{\partial p'}\langle p'|\alpha\rangle, \tag{B.13}$$

and hence

$$\langle \beta|x|\alpha\rangle = \int \mathrm{d}p'\, \phi_\beta^*(p')\, \mathrm{i}\hbar\frac{\partial}{\partial p'}\phi_\alpha(p'), \tag{B.14}$$

where $\phi_\alpha(p') = \langle p'|\alpha\rangle$.

13. Let

$$|\psi\rangle = 3\mathrm{i}\,|\phi_1\rangle - 7\mathrm{i}\,|\phi_2\rangle, \qquad |\chi\rangle = -\,|\phi_1\rangle + 2\mathrm{i}\,|\phi_2\rangle, \tag{B.15}$$

where $|\phi_1\rangle, |\phi_2\rangle$ are orthonormal. Find $|\psi + \chi\rangle$ and its bra, the two scalar products, and verify the Cauchy–Schwarz and triangle inequalities.

14. Discuss the Hermiticity of

$$A + A^\dagger, \qquad \mathrm{i}(A + A^\dagger), \qquad \mathrm{i}(A - A^\dagger), \tag{B.16}$$

find the adjoint of

$$f(A) = \frac{(I + \mathrm{i}A + 3A^2)(I - 2\mathrm{i}A - 9A^2)}{5I + 7A}, \tag{B.17}$$

and prove that expectation values of Hermitian (anti-Hermitian) operators are real (purely imaginary).

15. Show that $|\psi\rangle\langle\psi|$ is a projection operator only when $|\psi\rangle$ is normalized.

16. For

$$A = \begin{pmatrix} 5 & 3+2\mathrm{i} & 3\mathrm{i} \\ -\mathrm{i} & 3\mathrm{i} & 8 \\ 1-\mathrm{i} & 1 & 4 \end{pmatrix}, \quad |\psi\rangle = \begin{pmatrix} -1+\mathrm{i} \\ 3 \\ 2+3\mathrm{i} \end{pmatrix}, \quad \langle\phi| = \begin{pmatrix} 6 & -\mathrm{i} & 5 \end{pmatrix}, \tag{B.18}$$

compute $A\,|\psi\rangle$, $\langle\phi|\,A$, $\langle\phi|A|\psi\rangle$, and $|\psi\rangle\langle\phi|$; then compare complex conjugation, transpose, and Hermitian conjugation for the matrix, ket, and bra.

17. In a two-dimensional space let $A\,|\phi_1\rangle = |\phi_1\rangle$ and $A\,|\phi_2\rangle = -\,|\phi_2\rangle$, with A Hermitian and $|\phi_i\rangle$ orthonormal. For $B = |\phi_1\rangle\langle\phi_2|$, discuss Hermiticity, show $B^2 = 0$, show $BB^\dagger$ and $B^\dagger B$ are projectors, show $BB^\dagger - B^\dagger B$ is unitary, and show $C = BB^\dagger + B^\dagger B$ acts as the identity on both basis states.

18. Let $[A, A^\dagger] = I$ and

$$A\,|a\rangle = \sqrt{a}\,|a-1\rangle\,, \qquad A^\dagger\,|a\rangle = \sqrt{a+1}\,|a+1\rangle\,. \tag{B.19}$$

Evaluate $[A^\dagger A, A]$, $[A^\dagger A, A^\dagger]$, the stated ladder-operator matrix elements, and the diagonal matrix elements of $(A + A^\dagger)^2$ and $(A - A^\dagger)^2$.

19. Let

$$A = |\phi_1\rangle\langle\phi_1| + |\phi_2\rangle\langle\phi_2| + |\phi_3\rangle\langle\phi_3| - \mathrm{i}\,|\phi_1\rangle\langle\phi_2| - |\phi_1\rangle\langle\phi_3| \tag{B.20}$$
$$+\,\mathrm{i}\,|\phi_2\rangle\langle\phi_1| - |\phi_3\rangle\langle\phi_1|\,, \tag{B.21}$$

with a complete orthonormal three-state basis. Decide whether A is Hermitian, find A^2 and determine whether it is a projector, write its matrix, and find the eigensystem.

20. For

$$H = E\left(|\phi_1\rangle\langle\phi_1| - |\phi_2\rangle\langle\phi_2| - \mathrm{i}\,|\phi_1\rangle\langle\phi_2| + \mathrm{i}\,|\phi_2\rangle\langle\phi_1|\right), \tag{B.22}$$

find the Hermiticity, trace, matrix, eigensystem, and the commutators of H with $|\phi_1\rangle\langle\phi_1|$, $|\phi_2\rangle\langle\phi_2|$, and $|\phi_1\rangle\langle\phi_2|$.

21. Find conditions under which each operator is unitary:

$$U_1 = (I + \mathrm{i}A)(I - \mathrm{i}A)^{-1}, \qquad U_2 = (A + \mathrm{i}B)(A^2 + B^2)^{-1/2}. \tag{B.23}$$

22. A particle of mass m moves in an infinite well $0 < x < a$ and has

$$\psi(x,0) = \frac{A}{\sqrt{a}}\sin\frac{\pi x}{a} + \sqrt{\frac{3}{5a}}\sin\frac{3\pi x}{a} + \frac{1}{\sqrt{5a}}\sin\frac{5\pi x}{a}, \tag{B.24}$$

with real A. Normalize the state; give the energy outcomes and probabilities and the average energy; find $\psi(x,t)$; and find the probability of the time-dependent normalized fifth-level state

$$\phi_5(x,t) = \sqrt{\frac{2}{a}}\sin\frac{5\pi x}{a}\,\mathrm{e}^{-\mathrm{i}E_5 t/\hbar}. \tag{B.25}$$

23. In the same well, the source gives

$$\psi(x,0) = \sqrt{\frac{4}{5a}}\sin\frac{4\pi x}{a} + \sqrt{\frac{7}{5a}}\sin\frac{7\pi x}{a}. \tag{B.26}$$

Find $\psi(x,t)$, $\rho(x,t)$ and $J(x,t)$, and verify the continuity equation.

24. Consider

$$H = \epsilon_0 \begin{pmatrix} 1 & 0 & -1 \\ 0 & -1 & 0 \\ -1 & 0 & 1 \end{pmatrix}, \qquad A = a \begin{pmatrix} 0 & 4 & 0 \\ 4 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}. \tag{B.27}$$

Find the possible energy measurements. If the result $-\epsilon_0$ is obtained, find the possible subsequent A results, their probabilities, and ΔA.

25. The source prints

$$|\psi\rangle = \frac{1}{6}\begin{pmatrix} 1 \\ 0 \\ 4 \end{pmatrix}, \qquad A = \frac{1}{\sqrt{2}}\begin{pmatrix} 2 & 0 & 0 \\ 0 & 1 & \mathrm{i} \\ 0 & -\mathrm{i} & 1 \end{pmatrix}, \qquad B = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -\mathrm{i} \\ 0 & \mathrm{i} & 0 \end{pmatrix}. \tag{B.28}$$

Compare the probability for the sequential result $A = 0$ then $B = 1$ with that for $B = 1$ then $A = 0$, and decide whether the measurements are equivalent.

26. For the driven oscillator

$$H = \frac{P^2}{2m} + \frac{kX^2}{2} + qE_0 X \cos\omega t, \tag{B.29}$$

calculate $\mathrm{d}\langle X\rangle/\,\mathrm{d}t$ and $\mathrm{d}\langle H\rangle/\,\mathrm{d}t$, solve for $\langle X\rangle(t)$ subject to stated initial data, and determine the canonical momentum when the Hamiltonian is modified to

$$H = \frac{P^2}{2m} + \frac{kX^2}{2} + qE_0 X \cos\omega t + qB_0 P \sin\omega t. \tag{B.30}$$

27. If A is even and B is odd under parity P, evaluate PA^nP, PB^nP, and $P(AB)^3P$ for positive integer n.

28. For the SHO Hamiltonian

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2, \tag{B.31}$$

calculate $[H,[H,x^2]]$ and determine the relation between n_1, n_2 for which $\langle n_1|x^2|n_2\rangle \neq 0$.

29. An SHO is initially in

$$\psi(x,0) = N\sum_{n=0}^{\infty} c^n \psi_n(x), \tag{B.32}$$

where c is complex. Find $|N|$, the evolved state, the probability of return to the initial state, and $\langle H\rangle$ as functions of $|c|$.

30. A formal polar representation is stated as

$$a = \sqrt{N+1}\,\mathrm{e}^{\mathrm{i}\phi}, \qquad a^\dagger = \mathrm{e}^{-\mathrm{i}\phi}\sqrt{N+1}. \tag{B.33}$$

Starting with $[a,a^\dagger] = I$, calculate $[\cos\phi, N]$ and $\left\langle n_1\middle|\mathrm{e}^{\mathrm{i}\phi}\middle|n_2\right\rangle$.

31. An SHO is in the state

$$|\psi\rangle = \frac{|1\rangle + \lambda\mathrm{e}^{\mathrm{i}v}\,|2\rangle}{\sqrt{1+\lambda^2}}, \tag{B.34}$$

where the source describes $|1\rangle, |2\rangle$ as mutually orthogonal. Find $(\Delta x)^2$.

32. For $j = 1$, find the matrices of J_x, J_y, J_z in the $|j,m\rangle$ basis.

33. A simultaneous measurement of J^2, J_z gives $(j,m) = (0,0)$ with probability $3/4$ and $(1,-1)$ with probability $1/4$. Reconstruct the post-measurement state assuming no relative phase.

34. A spin-1 particle is in a uniform field $\boldsymbol{B} = B\hat{\boldsymbol{x}}$ with

$$H = g\boldsymbol{B}\cdot\boldsymbol{S}. \tag{B.35}$$

If the initial state is $|1,1\rangle$ in the S_z basis, write the evolved state in the S_x eigenbasis.

35. For $j = 3/2$ and

$$H = \frac{\alpha}{\hbar^2}(J_x^2 + J_y^2 - 2J_z^2) - \frac{\beta}{\hbar}J_z, \tag{B.36}$$

find the energy levels.

36. The supplied function is

$$\psi(x,y,z) = \sqrt{\frac{7}{16\pi}}\frac{z}{r^3}(5z^2 - 3r^2). \tag{B.37}$$

Using angular-momentum algebra, determine $Y_{3,1}$ and $Y_{3,-1}$ from this function.

37. Find all Clebsch–Gordan coefficients for adding $j_1 = 1$ and $j_2 = 1$, and express the coupled $|j, m\rangle$ states in the uncoupled basis.

38. For a qubit state

$$|\psi\rangle = \begin{pmatrix} \cos(\theta/2) \\ e^{i\phi} \sin(\theta/2) \end{pmatrix}, \tag{B.38}$$

write the density matrix in terms of a Bloch vector and Pauli matrices, extend to a vector of length r, identify the pure- and mixed-state conditions, and calculate $\langle \boldsymbol{\sigma} \cdot \hat{\boldsymbol{n}} \rangle$.

Reference texts

For further checking and alternative derivations, useful standard references are

- J. J. Sakurai and J. Napolitano, *Modern Quantum Mechanics*.
- R. Shankar, *Principles of Quantum Mechanics*.
- C. Cohen-Tannoudji, B. Diu and F. Laloë, *Quantum Mechanics*.